3D Graphene-Based Material as Catalyst Support Material for Fuel Cells

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Publication date:
2015

Document version
Accepted author manuscript

Citation for pulished version (APA):
Thrane Vindt, S. (2015). 3D Graphene-Based Material as Catalyst Support Material for Fuel Cells. Abstract from 5th International Workshop on Smart Materials and Structures, Marrakech, Morocco.

Smart Materials and Structures

5th International Workshop Marrakech

9. – 12. September 2015

FACHHOCHSCHULE KIEL
University of Applied Sciences

IMST
Institut für Werkstoff- und Oberflächentechnologie

Forschungs- und Entwicklungszentrum
Fachhochschule Kiel GmbH

THINFACE
European Training Network

Faculté des Sciences
Université Mohammed V

FST Marrakech

5th International Workshop on Smart Materials and Structures 2015, Marrakech-Morocco, September 9-12

Imprint
Published by: Institute for Materials & Surface Technology (IMST)
HAW Kiel-University of Applied Sciences
Grenzstrasse 3
D-24149 Kiel

Responsible of the content: Prof. Dr. M. Es-Souni

Kiel, August 2015

Dear colleagues,

Welcome to Marrakech for the 5th International Workshop on Smart Materials & Structures 2015 (SM&S 2015)!

The focus of this year's workshop is on Energy Materials.

Because of dwindling natural resources and the impact of fossil fuel on environment and global warming green energy is due to take a formidable share of up to 40% of the total energy mix in the next two decades. Reaching this target will partly depend on advances in energy materials and processes for green energy harvesting and storage. SM&S 2015 is bringing together researchers from Europe, Asia and Africa to discuss issues related to energy materials development and applications in a, hopefully, relaxed and pleasant atmosphere that should also promote networking and exchange of ideas.

For the scientific program we could gain the support of internationally renowned scientists for plenary and invited lectures. A common program of plenary lectures with the parallel conference "***International Meeting on Materials for Electronic Applications 2015"*** will permit to overview state of the art and perspectives of energy and multifunctional materials research. Progress reports are presented in parallel oral and poster sessions.

The poster sessions include very interesting presentations with a large number from Moroccan PhD students. We warmly encourage you to visit these sessions and discuss with the students.

We acknowledge the support of the local organizing committee, the symposia organizers and session chairs. We also acknowledge the supporting institutions and organizations: University of Applied Sciences Kiel,

Germany and F&E Zentrum FH Kiel GmbH, University Cadi Ayyad (Marrakech), especially the Faculty of Sciences and Technology and the Faculty of Sciences, University Mohammed V, Rabat.

We wish you a very good scientific meeting and a pleasant stay in Marrakech.

SM&S Chairs

Mohammed Es-Souni

Abdelilah Benyoussef

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Organization of the workshop

SM&S:

Mohammed Es-Souni*, Institute for Materials & Surface Technology, University of Applied Germany*

Abdelilah Benyoussef, *Royal Academy of Sciences & Faculty of Sciences, University Mohamed V, Rabat, Morocco*

OPV-Session organized by:

Prof. Horst-G Rubahn, *Nanosyd, Mads Clausen Institute, University of Southern Denmark*

Prof. Morten Madsen, *Nanosyd, Mads Clausen Institute, University of Southern Denmark*

Publications: Peer reviewed papers will be published in a special issue of Applied Physics A.

SM&S International Advisory Board:

- Prof. Pooi See Lee, *School of Materials Science & Engineering, Nanyang Technological University, Singapore*
- Prof. Horst-G Rubahn*, Nanosyd, Mads Clausen Institute, University of Southern Denmark*
- Dr. Mato Knez, *Ikerbasque Research Professor, Nanomaterials Group Leader, San Sebastian (Spain)*
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- Dr. Aline Rougier, *Institut de Chimie de la Matière Condensée de Bordeaux, Université de Bordeaux, France*
- Prof. Soshu Kirihara, *Osaka University, Japan*
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- Prof. Nagahiro Saito, *Nagoya University Graduate School of Engineering, Materials, Physics and Energy Engineering, Japan*

SM&S Session Chairs

Energy Storage	T. Sritharan
Smart Materials and Devices	A. Douhal
Solar Cells	M. Es-Souni
Energy Materials	N. Saito
Organic Solar Cells	M. Krunks
Processing	S. Kirihara
Properties and Applications	M. Knez
Numerical Studies	J. Adam
Ferroic Materials and Structure	A. Benyoussef
Plenary Sessions	M. Es-Souni, A. Douhal, V. Dyakonov

Local Committee, Marrakech

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- Prof. Youssef El Amraoui, Physics DPT, University Mohamed V, Rabat, Morocco
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- Prof. M'Barek Amjoud, Chemistry DPT, Cadi Ayyad University, Marrakech

Secretariat:

Conference website SM&S: www.workshop-smartmaterials.com

E-mail: info@workshop-smartmaterials.com

SM&S Program

The scientific program of SM&S consists of 56 contributions:

7 Plenary talks (SM&S and IMMEA)
14 Invited talks
23 Contributed talks
42 Posters

Information for participants

Conference Venue

Faculté des Sciences et Techniques
B.P 549, Av.Abdelkarim Elkhattabi, Guéliz Marrakech

Allocation of conference rooms and poster session

The conference rooms are numbered (Lecture Hall 1 and 2 and seminar room 1). The sessions are scheduled as displayed in the conference program.

The poster sessions take place in the foyer.

Presentations

The workshop language is English.

Oral presentations

It is recommended to use electronic presentation technique (i.e. pdf files, Power Point, Impress or similar). Projectors, notebooks, and video switches are provided in the conference rooms. Please upload your presentation before session start and check the presentation with the room attendant.
Abbreviations:

P	Plenary talk:	45 min, including discussion
I	Invited talk:	30 min, including discussion
T	Talk:	20 min, including discussion

Poster presentations

2 poster sessions are scheduled Thursday and Friday after the oral talk programs.
The necessary material for mounting the posters will be provided. There will be an attendant for help. The preferable poster size is A0 (ISO / DIN). The width of a poster should not exceed 90 cm.

Conference Service

Workshop office

The workshop office opens Wednesday, September 9, from at 16.00 – 20.00h and Thursday morning at 8.00 h. On registration the participants, who have not yet paid the registration fee, are requested to pay the respective amount in cash. All full participants then receive their name-tags, lunch and dinner tickets and, upon request, a payment receipt with confirmation of participation. The name-tags should be worn visible during the entire workshop.
Coffee, lunch, and Workshop dinner are included in the registration fee for full participants.

Internet access

Access to the internet WLAN will be available.

Message board

Program changes and important information will be announced at the workshop office.

Coffee, Lunch

Coffee

Coffee and tea will be supplied during the session breaks.

Lunch and Workshop dinner

For lunch and the Workshop dinner every full participant has received 3 lunch tickets and 1 dinner ticket when registering at the Workshop office.

Conference program Smart Materials and Structures

Welcome, Wednesday, 2015-09-09	
16.00	Arrival Workshop office opened
19.00	Welcome

Morning session, Thursday, 2015-09-10	
8.30	**Opening**
	Plenary Talks Room: Lecture hall 1
9.00 P	*Catherine Dubourdieu, France* Towards complex oxide electronics on semiconductors
9.45 P	*Andrew Gallant, UK* Micro- and Nanoengineering of Plasmonic Terahertz Devices
10.30 – 10.50	Break: Coffee / Tea
10.50 – 12.40	**Energy Storage** Chair: Thirumany Sritharan Room: Lecture hall 2
10.50 I	*Mato Knez, Spain* Optimization of supercapacitor electrodes by Atomic Layer Deposition
11.20 I	*Rose-Noelle Vannier, France* Oxide ion transport in Mixed Ionic Electronic Conductors as SOFC cathodes
11.50 I	*Jean-Claude Badot, France* The contribution of the dielectric spectroscopy to the multiscale study of the electrode materials cells
12.20 T	*Eivind Skou, Denmark* The “Missing Buffer Effect” and the implications for super capacitors using aqueous electrolytes
12.45 – 14.00	**Lunch break**

Afternoon sessions, Thursday, 2015-09-10	
	Plenary Talk Room: Lecture hall 1
14.00 P	*Valerii Vinokur, USA* Vortex Mott insulator-metal transitions: experiment and theory Chair : Catherine Dubourdieu
14.50 – 16.20	**Smart Materials and Devices** Chair: Abderrazzak Douhal Room: Lecture hall 2
14.50 I	*Aline Rougier, France* Electrochromics as smart materials
15.20 I	*Franz Faupel, Germany* Functional Nanocomposites – From Fabrication to Function
15.50 I	*Mimouna Baitoul, Morocco* Graphene derivatives based nanocomposites for potential applications
16.20 – 16.40	Break: Coffee, Tea
16.40 – 18.00	**Solar Cells** Chair: Mohammed Es-Souni Room: Lecture hall 2
16.40 I	*Thirumany Sritharan, Singapore* Iron Pyrite (FeS_2) Nanoparticles and Thin Films as Photon Absorbers and Counter Electrodes in Solar Cells
17.10 I	*Malle Krunks, Estonia* Metal oxide and metal sulphide nanostructures by solution methods
17.40 T	*Karima Meziane, Morocco* Study of the physical properties of zinc oxide thin films prepared by the solgel method and doped lithium for photovoltaic applications
18.00 – 19.00	Poster session I

Morning session, Friday, 2015-09-11	
	Plenary Talks Room: Lecture hall 1
8.30 P	*Abderrazzak Douhal, Spain* Ultrafast Dynamics in Metal-Organic-Frameworks (MOFs) Chair: Aline Rougier
9.15 P	*Dagou Zeze, UK* Nanostructured Materials & Devices Chair : Arunas Krotkus
10.00 – 10.20	Break: Coffee / Tea
10.20 – 12.30	**Energy Materials** Chair: Nagahiro Saito Room: Lecture hall 2
10.20 I	*Soshu Kirihara, Japan* Stereolithographic Additive Manufacturing of Ceramics Dendrites with Geometric Fluctuations for Energy and Material Flows Modulation
10.50 I	*Minoru Mizuhata, Japan* Enhancement of photoluminescence and electrochemical activity in porous silicon/metal oxide composite materials
11.20 I	*Michel Latroche, France* Alloying and size effects on the sorption properties of Mg-based hydrides
11.50 T	*Maryem El Khatabi, Morocco* An in-depth study of the effect of transition metals on the hydrogen storageproprieties of MgH_2
12.10 T	*Andreas Zeinert, France* Optical and photocatalytic properties of $BiVO_4$ thin films
12.45 – 14.00	**Lunch break**

Afternoon sessions, Friday, 2015-09-11			
	Plenary Talk Chair: Horst-Günter Rubahn Room: Lecture Hall 1		
14.00 P	*Vladimir Dyakonov, Germany* Recombination pathways in high efficiency organic solar cells		
14.50 – 16.20	**Organic Solar Cells** Chair: Malle Krunks Room: Seminar room 1	14.50 – 16.10	**Processing** Chair: Soshu Kirihara Room: Lecture hall 2
14.50 I	*Jost Adam, Denmark* Modeling nanostructure-enhanced light trapping in organic solar cells	14.50 I	*Nagahiro Saito, Japan* Solution Plasma Process for Fine Nanoparticles and Carbon Materials Production
15.20 T	*Vida Engmann, Denmark* Stabilization of Organic Solar Cells by Ternary Blending Active Layers with Additives	15.20 I	*Mady Elbahri, Germany, Finland* Macroscopic optical antennas with glassy disordered dipolar composites
15.40 T	*Hajar Jaouani, Morocco* Organic Solar Cells integrated in Smart Textile	15.50 T	*Nele Berger, Germany* On-substrate fabrication of porous Al-oxide templates with tunable pore diameters and interpore distances
16.00 T	*Morten Madsen, Denmark* Application of non-crystalline MoO_x films for optoelectronic organic devices		
16.20 – 16.40	Break: Coffee / Tea		

16.40 – 18.00	**Properties and Applications** Chair: Mato Knez Room: Lecture hall 2	16.40 – 18.00	**Numerical Studies** Chair: Jost Adam Room: Seminar room 1
16.40 T	*Dimitri Schopf, Germany* Supported porous carbon and carbon-CNT-nanocomposites for supercapacitor applications	16.40 T	*Houda Ennaceri, Morocco* Optical Performance of ZnO and ZAO (ZnO:Al) Thin Films prepared by Reactive Magnetron Sputtering: Experimental and ab initio Study
17.00 T	*Boubker Ouadil, Morocco* Preparation of antibacterial and conductive textiles impregnated with graphene oxide, graphene and metallic nanoparticles	17.00 T	*Abderrahmanan Abbassi, Morocco* First principles study on the electronic and optical properties of Si and Al co-doped zinc oxide for solar cell devices
17.20 T	*Albert Juma, Botswana* Effect of microstructure on the electrical properties of TiO_2 thin films deposited by chemical spray pyrolysis	17.20 T	*Mourad Boujnah, Morocco* Ab initio comparative study of Scintillating Crystals LaX_3 with X=(F, Br and I) using mBJ exchange-correlation potential
17.40 T	*Ghizlan El Hallani, Morocco* *Effect of different molarities on structural and optical properties of ZnO thin films elaborated by spin coating method*	17.40 T	*Imane Matrane, Morocco* *Numerical study of the adsorption and the diffusion on the clean (1×1) unreconstructed and (1×2), (1×3) and (1×4) reconstructed Pt (110) surfaces*

18.00 – 19.00	Poster session II
19.00	Departure to conference party

Saturday, 2015-09-12	
9.00 – 11.40	**Ferroic Materials and Structure** Chair: Abdelilah Benyoussef Room: Lecture hall 2
9.00 T	*Jaroslavas Belovickis, Lithuania* Ferroelectric and ultrasonic studies on polymer based P(VDF-TrFE) composites with PZT, BTO and CFO inclusions
9.20 T	*Meriem Ben Ali, Morocco* Structural and magnetic properties of mixed Mn–Zn ferrites nanoparticles synthesized by Sol/Gel method
9.40 T	*Khadija El Maalam, Morocco* Composites perovskites materials for magnetic refrigeration application
10.00 T	*Mohamed Azrour, Morocco* Crystal structure and room and high temperature raman spectroscopy studies of $M_{3-x}M'_xX_2O_8$ (M = Ba, Sr; M' = Pb, Sr; X = P, As, V; $0 \leq x \leq 3$) and $A_{1-x}A'_xPb_4(XO_4)_3$ (A = Na, K; A' = Ag, K; X = P, As, V and $0 \leq x \leq 1$)
10.20 T	*Abdehalim Elbasset, Morocco* Impedance complex, dielectric relaxation and electrical conductivity studies of $Ba_{1-x}Sr_xTiO_3$ ceramics
10.40 – 11.00	Break: Coffee / Tea
11.00 T	*Abdelhak El Ghandouri, Morocco* Structural and electrical properties of sol-gel processed strontium – doped barium titanate ceramics
11.20 T	*Omar Oabi, Morocco* High Seebeck Coefficients in $ZnO\text{-}P_2O_5$/ (Ni & Co) Composites
	Plenary Talk Room: Lecture Hall 1
11.50 P	*Pooi See Lee, Singapore* High Performance Hybrid Pseudocapacitive Materials for Energy Storage Chair: Mohammed Es-Souni
12.35	Closure
12.45 – 14.00	Lunch

List of Poster Presentations

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P1	*Ibtissam El Housni, Morocco* Energy and exergy analysis of an integrated solar combined cycle system (ISCCS) in Morocco
P2	*Arkadiusz Goszczak, Denmark* Nanostructures for organic solar cells from anodized aluminum templates
P3	*Sara Mtougui, Morocco* Simulating the feasibility of installing a smart grid in Rabat, Morocco
P4	*Nabil Chakhchaoui, Morocco* Use of electro-active polymers in the energy harvesting application to TTU
P5	*Zineb Sabri, Morocco* Effect of different signals of polarization using electrostrictive polymers for harvesting energy
P6	*Steffen Thrane Vindt, Denmark* 3D graphene-based material as catalyst support material for fuel cells
P7	*Abdelilah Lahmar, France* Temperature influence on microstructure and optical properties of TiO_2-Au monolayer thin films
P8	*Abdehalim Elbasset, Morocco* Investigation of the structural, microstructural and optical properties of strontium titanate$SrTiO_3$
P9	*Hicham Gounaya, Morocco* The relaxation and the diffusion of Au and Pt adatoms on missing row reconstructed surfaces of gold

P10	*Chahrazed Kaddour, Algeria* Thermal effects on I-V characteristics for GaAs MESFET devices
P11	*Ali Hafs, Algeria* Structural characterization and superconducting properties of Nb_3Al by combustion synthesis
P12	*Yusuke Kondo, Japan* Encapsulation of gold nanoparticles onto green tea extracts-modified chitosan flakes as catalyst for 4-nitrophenol Reduction
P13	*Najoua Zayyoun, Morocco* PH effect on the synthesis of Cu_2O/CuO nanoparticles by sol-gel method in a glycolic medium
P14	*Yoshida Shuhei, Japan* Preparation and catalytic evaluation of natural leaf supported gold nanoparticles
P15	*Hyemin Kim, Japan* Simple one-step synthesis of nanostructured MnO_2 colloidal suspension by plasma discharge in liquid
P16	*Anyarat Watthanaphanit, Japan* Synthesis of black titania spheres with efficient visible-light photocatalytic activity by water plasma
P17	*Sana El-Kacemi, Morocco* Photocatalytic degradation of methylorange by TiO_2 nanostructured thin films
P18	*Abdessamad Moumen, Morocco* Synthesis of nickel nanoparticles in aqueous copolymer emulsion
P19	*Mohamed Houmad, Morocco* Absorption of visible light by GaAs and GaN nanosheet

No.	Poster session II 2015-09-11
P1	*Rabab Bekkari, Morocco* Influence of sol concentration and annealing temperature on the structural and optical properties of nanocrystalline ZnO thin films synthesized by the sol-gel method
P2	*Chaki Imane, Morocco* Physical properties of Gd doped ZnO thin films grown by spray pyrolysis
P3	*Klaa Kalthoum, Algeria* Structural, electronic and thermal properties of wurtzite ZnO structure
P4	*Mohamed Khuili, Morocco* First principles study of (Mg,Al)-codoped ZnO with GGA and mBJ approximations
P5	*Abdi Naima, Algeria* First principles calculations of the structural, elastic and thermal properties of ZnO in zinc blende structure
P6	*Bhihi Mohamed, Morocco* First principal study of hydrogen storage proprieties of double substituted Mg based hydrides $Mg_{14}TMLiH_{32}$, (TM = Sc, Ti, V, Cr, Y, Zr, Nb, Mo)
P7	*Mustapha Abdellaoui, Morocco* Ab initio study of effects of B (Bsub,Bins) substituted and insertion Tm (Sr,Ca) co-doping on destabilizing of MgH_2
P8	*Zakaryaa Zarhri, Morocco* First principal calculations of optical and electrical properties in F and Al doped TiO_2 DMS
P9	*Mohamed Tadout,Morocco* First principles calculations of GaN and AlN nanosheets

No.	Poster session II 2015-09-11
P10	*Karim Saidi, Morocco* Numerical simulation of the filling phase of the microinjection process with the level set method
P11	*Ahmed Moussaoui, Morocco* Numerical study by the meshless method LRPIM of shape parameter in radial basis function in linear elasticity
P12	*Omar El Rhazouani, Morocco* Antisite disorder study by Monte Carlo Simulation of the double perovskite Sr_2CrReO_6
P13	*Abderrahmanan Abbassi, Morocco* Spontaneous polarization, magnetic and electronic properties of $BiXO_3$(X=Co, Mn, Fe, V, Zn) : First principles study
P14	*Mohssine El Bachra, Morocco* Magnetic properties of heavy fermions compound URu_2Si_2: ab initio calculations and Monte Carlo simulation
P15	*Rachid Masrour, Morocco* Magnetism of size effect in graphene nano-islands: A Monte Carlo study
P16	*Younes Benhouria, Morocco* Dynamic compensation temperatures and hysteresis behaviors of a mixed spin Ising double walled ferromagnetic nanotubes
P17	*Dani Ibtissam, Morocco* Phase diagrams of spin-1 Ashkin-Teller model with crystal field and transverse field
P18	*Khadija El Maalam, Morocco* Changing the magnetic and optical properties of (Ga, Fe)N and (Ga, Co)N by alloying with oxygen

No.	Poster session II 2015-09-11
P19	*Abderrahim Ait Raiss, Morocco* Magnetic and magneto-optical properties of doped and co-doped CdTe
P20	*Younes Sbai, Morocco* Magnetic properties and phase transition in transitions metal doped semiconductor GaN
P21	*Zakaria Mahhouti, Morocco* Structural and magnetic study of $Co_{(1-x)}Ni_xFe_2O_4$ nanoparticles synthesized by the sol-gel method
P22	*Hassan El Moussaoui, Morocco* Synthesis and magnetic properties of cobalt ferrite nanoparticles doped with neodymium and tin
P23	*Ali Oubelkacem, Morocco* Thermodynamic properties and hysteresis behaviors of a mixed ferrimagnetic nanowire

Program

SM&S

Morning sessions

Thursday, September 10th, 2015

Energy Storage

Time: 10.50 – 12.40

Room: Lecture hall 2

Chair: Thirumany Sritharan

Thursday, 2015-09-10	10.50	Invited talk	Energy storage	Lecture hall 2

Optimization of Supercapacitor Electrodes by Atomic Layer Deposition

Fan Yang[1], Lianbing Zhang[1], Ana Zuzuarregui Olasagasti[1], Keith Gregorczyk[1], Le Li[1], Mikel Beltrán[1], Christopher Tollan[1], Andrey Chuvilin[1,2] and Mato Knez[1,2]

[1]CIC nanoGUNE Consolider, Tolosa Hiribidea 76, 20018 Donostia-San Sebastian, Spain
[2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain

Graphene is a material with exciting physical properties and therefore of great interest for numerous applications including, but not limited to electronics, energy storage and conversion, etc. Although meanwhile vapor based synthetic processes for defect-free graphene have been established, wet chemical procedures that yield graphene oxide (GO) are most common. The drawback of those materials is their large number of defects, commonly oxidized carbon, that have serious negative impact on the physical or electrochemical properties of this graphitic compound. The chemical reduction of such defects is a common procedure and yields reduced graphene oxide (rGO) that, in spite of still having defect sites, closely resembles the properties of graphene. Functionalization of the remaining defect sites with precise control may be of great benefit for any anticipated application and pave ways for novel graphene-based devices with high efficiency.

In this work, we demonstrate how such ultimately efficient functionalization can be achieved, namely through controlled binding of very small amount of materials such as RuO_2 to rGO by atomic layer deposition (ALD) and in this way substituting the native defect sites with RuO_2 defects. On the example of a supercapacitor, we show that the defect functionalization results in significantly enhanced specific capacitance of the electrode, and that its energy density can be stabilized even at high consumption rates.

Thursday, 2015-09-10	11.20	Invited talk	Energy storage	Lecture hall 2

Oxide Ion Transport in Mixed Ionic Electronic Conductors as SOFC Cathodes

Rose-Noelle Vannier

Unité de Catalyse et de Chimie du Solide, Université de Lille, UMR CNRS 8181, ENSCL, 59652 Villeneuve d'Ascq Cedex, France

A Solid Oxide Fuel Celle (SOFC) is based on an oxide ion conductive ceramic used as electrolyte which separates two compartments, one containing air and the other one the fuel which can be hydrogen or a hydrocarbon such as methane. Due to the difference of oxygen chemical potential between the two compartments, oxygen molecules are reduced into oxide ions at the cathode which migrate through the electrolyte to react with hydrogen to produce water and electricity. At the cathode, the strontium substituted lanthanum manganite ($La_{1-x}Sr_xMnO_{3-\delta}$) has been widely studied as cathode. However, despite a high catalytic activity, its electrical conductivity is mainly electronic which restrains the Oxygen Reduction Reaction (ORR) to the triple point boundary at the interface between the gas phase, the electrode and the electrolyte. In this frame, Mixed Ionic Electronic Conductors (MIEC) are usually preferred to allow the ORR to be sprayed on the whole electrode volume and not only at the electrode/electrolyte interface. Among these, cobaltites are promising but exhibit high thermal expansion coefficient which may be mechanically incompatible with the commonly used electrolytes.

Here, after a brief introduction on the main materials studied as SOFC cathode with a focus on the materials currently studied at UCCS, the characterisation of the oxide ion transport in such ceramics will be described.

Thursday, 2015-09-10	11.50	Invited talk	Energy storage	Lecture hall 2

The Contribution of the Dielectric Spectroscopy of the Multiscale Study of the Electrode Materials

Jean-Claude Badot[1], Olivier Dubrunfaut[2] and Bernard Lestriez[3]

[1]Institut de Recherche de Chimie Paris, UMR CNRS 8247, Réseau sur le Stockage Electrochimique de l'Energie (RS2E), Chimie ParisTech, 11 rue P. et M. Curie 75231 Paris Cedex 05, France
[2]Group of electrical engineering - Paris (GeePs), UMR CNRS 8507, CentraleSupelec, Sorbonne
Universites, UPMC Univ Paris 06, Univ Paris-Sud, 11 rue Joliot-Curie, 91192 Gif-sur-Yvette, France
[3]Institut des Matériaux Jean Rouxel, UMR CNRS 6502, Université de Nantes, 2 rue de la Houssinière, BP32229, 44322 Nantes, France

The improvement of battery performance requires the rationale optimization of the composite electrode. The developments of new experimental techniques as well as methodologies are needed to understand the relationships between the composition, the architecture and the performance of composite electrodes. The fruitful contribution of Broadband Dielectric Spectroscopy (BDS) to study hierarchical materials applied to lithium ion and lithium metal batteries electrodes has been previously shown [1-5]. The results demonstrate that the broadband dielectric spectroscopy technique is very sensitive to the different scales of the electrode architecture involved in the electronic transport, from interatomic distances to macroscopic sizes, as well as to the morphology at these scales, coarse or fine distribution of the constituents. When the frequency increases, different kinds of polarizations appear from macroscopic sizes to interatomic distances (Fig. 1) and give rise to dielectric relaxations in the following order: (a) space-charge polarization (low-frequency range) due to the interface sample/current collector; (b) polarization of clusters (or agglomerates) of particles (micronic scale) and (c) polarization of particles due to the

existence of resistive junctions between them; d) electron transfers (nanometric or interatomic scale).

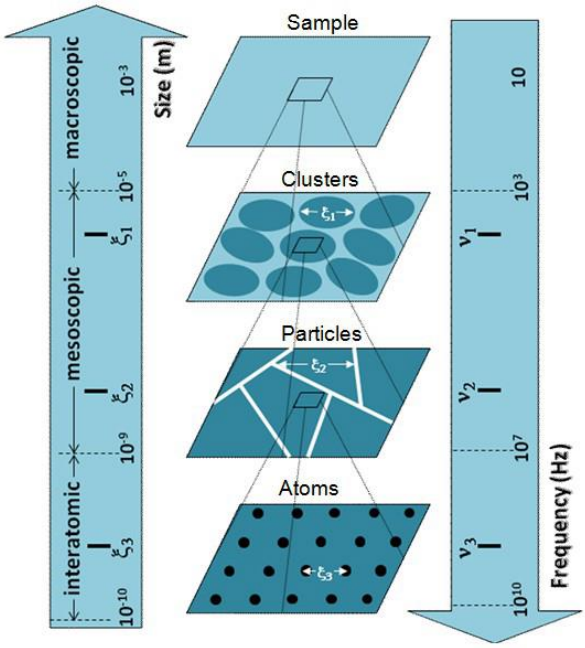

Fig. 1 Schematic description of a hierarchical architecture at different scales of a powdered material: different sources of polarizations vs. frequency and size.

The BDS measurement was up to now ex situ measurement, on dry electrode. They provide a fundamental insight into the conduction properties at all scales of the materials before being integrated in a real battery. An innovative device (measurement cell) has been developed to make synchronized BDS measurements and electrochemical cycling. The frequency range is about 103 - 1010 Hz. In this work, data acquisitions were made on dry electrodes (Active material / Carbon black / PVdF) and then on the same electrode wetted with an electrolyte. Short- and long-range motions of ions are evidenced in the low-frequency region. At higher frequencies, the study shows for the first time the influence of the ions of the electrolyte on the transfer of the electronic charges (and conversely) at the micronic and nanometric scales.

Thursday, 2015-09-10	11.50	Invited talk	Energy storage	Lecture hall 2

[1] J.C. Badot, E. Ligneel, O. Dubrunfaut, D. Guyomard, and B. Lestriez, Adv. Funct. Mater. 2009, 19, 2749.
[2] J.C. Badot, E. Ligneel, O. Dubrunfaut, J. Gaubicher, D. Guyomard, B. Lestriez, Phys. Chem. Chem. Phys. 2012, 14, 9500.
[3] K.A. Seid, J.C. Badot, O. Dubrunfaut, S. Levasseur, D. Guyomard, B. Lestriez, J. Mater. Chem. 2012, 22, 2641.
[4] K.A. Seid, J.C. Badot, O. Dubrunfaut, S. Levasseur, D. Guyomard, B. Lestriez, J. Mater. Chem. 2012, 22, 24057.
[5] K.A. Seid, J.C. Badot, C. Perca, O. Dubrunfaut , P. Soudan , D. Guyomard, B. Lestriez. Adv. Energy Mater. 2015, 5, 1400903.

Thursday, 2015-09-10	12.20	Talk	Energy storage	Lecture hall 2

The “Missing Buffer Effect” and the Implications for Super Capacitors using Aqueous Electrolytes

Steffen Thrane Vindt and Eivind M. Skou

Department of Chemical Engineering, Biotechnology and Environmental Technology, University Of Southern Denmark, DK-5230 Odense M, Denmark

When an aqueous solution of neutral salt is used as electrolyte in a super capacitor in contrast to an acid or alkaline solution an extended potential window is sometimes observed.

In the present work this phenomenon has been investigated systematically using high surface porous carbon electrodes and unbuffered as well as buffered aqueous solutions as electrolytes.

It is shown that the effect is caused by initial hydrogen production at the low potential limit and initial oxygen evolution at the high potential limit. Due to pH effects associated with hydrogen and oxygen formation the potential limits will be extended, when a specific current limit is used to define the potential window.

Due to the energy dependence of the square of the charge potential the energy content of a super capacitor under dynamic load may be increased by as much as 50% due to this “missing buffer effect”.

Afternoon sessions

Thursday, September 10th, 2015

Smart Materials and Devices

Time: 14.50 – 16.20

Room: Lecture hall 2

Chair: Abderrazzak Douhal

Thursday, 2015-09-10	14.50	Invited talk	Smart materials and devices	Lecture hall 2

Electrochromics as Smart Materials

Aline Rougier

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In respect of their adaptability and performance, electrochromic devices, ECDs, which are able to change their optical properties under an applied voltage, have received significant attention. Target applications are multifold, both in the visible (automotive sunroofs, smart windows, ophthalmic lenses, domestic appliances...) and in the infrared region (satellites thermal control, IR furtivity). In a standard configuration, ECDs, also described as optical batteries, are based on a 5 layers stack, schematized by TCO/EC/Electrolyte/CE/TCO, in which TCO stands for Transparent Conducting Oxides, EC for Electrochromic material and CE for Counter Electrode. In the group, aiming at improving materials and devices in respect of specific applications modified NiO [1] thin films as counter electrode, ZnO based thin films as transparent conducting layer [2] WO_3 [3] and PEDOT electrochromic layers are particularly studied. In this presentation, we will discuss how we can (i) modulate the materials characteristics in terms of morphology, composition, structure, (ii) adapt the synthesis process to the substrate nature, considering paper, plastic, glass or metal substrate, (iii) evidence new electrochemical reactivity in ionic liquid based electrolytes and (iv) optimize the device architecture in order to improve the ECDs performances.

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Thursday, 2015-09-10	14.50	Invited talk	Smart materials and devices	Lecture hall 2

[2] Low Temperature Transparent Conducting Oxides based on Zinc Oxide Thin Films. J. Clatot, G. Campet, A. Zeinert, C. Labrugère, M. Nistor, and A. Rougier, Solar Energy Materials and Solar Cells, 95(8), 2357-2362 (2011).
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Thursday, 2015-09-10	15.20	Invited talk	Smart materials and devices	Lecture hall 2

Functional Nanocomposites – From Fabrication to Function

Franz Faupel[1], Sebastian Zabel[1], Thomas Strunskus[1], Oleksandr Polonskyi[1], and Mady Elbahri[2,3]

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Highly filled particulate nanocomposite films consisting of metal nanoparticles in a dielectric organic or ceramic matrix have unique functional properties with hosts of applications [1]. The present talk demonstrates how vapor phase deposition techniques can be employed for tailoring the nanostructure and the resulting properties. Vapor phase deposition, inter alia, allows excellent control of the metallic filling factor and its depth profile as well as the incorporation of alloy nanoparticles with well-defined composition. We applied various methods such as sputtering, evaporation, and plasma polymerization for the deposition of the matrix component, while the metallic components were mostly sputter-deposited or evaporated. Moreover, a high-rate gas aggregation cluster source was utilized to obtain independent control of filling factor and size of the embedded nanoparticles. Examples include optical composites with tuned particle surface plasmon resonances for plasmonic applications [2,3], magnetic high frequency materials with cut-off frequencies well above 1 GHz [4], sensors [5] and photoswitchable devices [6] that are based on the huge change in the electronic properties near the percolation threshold, and biocompatible antibacterial coatings with tailored release rate [7]. In addition to the

particulate composites, it will be shown how magnetoelectric layered composites consisting of magnetostrictive and piezoelectric layers can be explored as low frequency magnetic field sensors with sensitivities down to the pT range [8]. Finally, a new concept of a robust, fully integrable, broad band magnetic field sensor based on the delta E effect will be presented [9,10].

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Thursday, 2015-09-10	15.50	Invited talk	Smart materials and devices	Lecture hall 2

Graphene Derivatives Based Nanocomposites for Potential Applications

M. Baitoul

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Carbon nanomaterials such as carbon nanotubes and more recently graphene have attracted significant interest of chemist and physicist due to their exceptional electronic and structural properties. Structurally modifying graphene, by chemical or physical functionnalization, reveals numerous possibility of tuning its band gap and properties which open the way for its use in various applications. We report here different methods of functionnalization of graphene derivatives with nanostructured materials and polymers and their optical properties. Optical, Steady state and time resolved Photoluminescence investigations on Graphene layers decorated with nanostructured porphyrin showed charge/energy transfer and modulation of their band gap and emission. While nanostructured oxides were grown successfully on graphene derivatives such as graphene oxide and reduced graphene oxide layers showing novel optoelectronic properties and promising potential for white light emitting diodes and energy.

Solar Cells

Time: 16.40 – 18.00

Room: Lecture hall 2

Chair: Mohammed Es-Souni

Thursday, 2015-09-10	16.40	Invited talk	Solar cells	Lecture hall 2

Iron Pyrite (FeS_2) Nanoparticles and Thin Films as Photon Absorbers and Counter Electrodes in Solar Cells

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Iron pyrite (FeS_2) has a high light absorption coefficient ($\alpha > 10^5$ cm^{-1} for hv > 1.3 eV) and a suitable bandgap (Eg~0.9-1.0 eV) for photovoltaic applications but its poor performance in experimental cells has precluded its use until now. This is attributed to impurity phases and defects. Synthesis of pure pyrite nanoparticles by a hot injection method was investigated to understand the effects of synthesis parameters on the initial monomer concentration, nanoparticle size, morphology and the structure. It was shown that nanoparticles of shapes such as cube, plate and sphere could be produced by changing the synthesis parameters. In particular, the coarsening mechanism of the cubes and plates were investigated in detail and were found to be different to that of the spheres. Cubes and plates were found to form by a method of aggregation of nano-sized, quantum dots.

Iron pyrite films were prepared and tested as counter electrodes in a dye sensitized solar cell. The different shapes of NPs were made into films on a conducting substrate and tested as Counter Electrodes in Dye Sensitized Solar Cells based iodide electrolyte. They were found to give a power conversion efficiency of 5.2-7.6 %, comparable to Pt which gave 7.9% in an iodide electrolyte based cell. Counter electrodes made from spray pyrolysed films gave slightly higher efficiency and also worked with Co-based electrolyte. Cyclic voltammetry and impedance spectroscopy showed that the catalytic activity of the particles is comparable to that of Pt. The potential reasons for this will be discussed.

Thursday, 2015-09-10	16.40	Invited talk	Solar cells	Lecture hall 2

Such excellent performance of pyrite counter electrode makes it a potential electrode material in dye sensitized solar cells.

This work is part of the SinBeRISE CREATE program funded by the National Research Foundation of Singapore and is done in collaboration with the University of California, Berkeley and National University of Singapore.

Thursday, 2015-09-10	17.10	Invited talk	Solar cells	Lecture hall 2

Metal Oxide and Metal Sulphide Nanostructures by Solution Methods

Malle Krunks

Department of Materials Science, Tallinn University of Technology, Tallinn, Estonia

The preparation and properties of novel ZnO nanostructures (nanorods, nanoneedles, hierarchical nanorods and scrolled nanobelts) and ZnS nanorod arrays made by simple, robust and non-vacuum chemical spray pyrolysis method will be introduced.

ZnO nanostructures are grown on glass and/or polymeric substrates using aqueous or alcohol based solutions of zinc salts [1]. ZnS nanorod layers are obtained by spray using thiourea as sulphur source in addition to a zinc salt in spray solution [2]. Solution is pulverised in form of fine droplets onto a preheated substrate. The morphology of ZnO, ZnS nanorod layers, dimensions and orientation of crystals are controlled by the growth temperature, precursor concentration and additives in the spray solution which may retard the crystal lateral growth. The density of nucleation centres on the substrate or seed layer is the key parameter controlling the aspect ratio of the rods and morphology of the nanostructured layers. The growth and nucleation mechanisms of ZnO nanorods and scrolled nanobelts, and the formation of hierarchical nanostructures will be discussed.

Light harvesting ability of ZnO and ZnS nanostructures as well as the possibilities to increase the light absorption in the materials and devices via surface plasmon resonance effect will be discussed. Gold and silver nanoparticles are produced by solution methods of spray or spin coating. In both cases nanoparticles form upon the thermal decomposition of precursors. Nanoparticle size and distribution on the

substrate is controlled by the solution concentration and substrate temperature. The surface plasmon resonance effect caused by noble metal nanoparticles is used to modify light absorption in metal oxide and sulphide films and nanostructured layers. Examples on improved light harvesting in thin film solar cells and effect on the cell output properties will be introduced.

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Study of the Physical Properties of Zinc Oxide Thin Films Prepared by the Sol-Gel Method and Doped Lithium for Photovoltaic Applications

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ZnO is a very promising material for semiconductor device applications. It has a direct and wide band gap in the near-UV spectral region and a large free-exciton binding energy (60Mev) so that excitonic emission processes can persist at or even above room temperature. ZnO crystallizes in the wurtzite structure, the same as GaN, but, in contrast, ZnO is available as large bulk single crystals. Its properties have been studied since the early days of semiconductor electronics, but the use of ZnO as a semiconductor in electronic devices has been hindered by the lack of control over its electrical conductivity: ZnO crystals are almost always n-type, the cause of which has been a matter of extensive debate and research.

A number of different techniques have been utilized to prepare ZnO thin films such as chemical vapor deposition, magnetron sputtering and sol-gel method. Among these methods, the sol-gel method process an attractive technique for obtaining thin film, due to controllability of compositions, simple facilities, low cost, etc. In the present work, we investigated effects of Li structure and properties of ZnO films. The realization of P-type ZnO is difficult, owing to factors such as self_compensating defects ,deep acceptor level and low solubility of acceptor dopants. The lithium is a good candidate for producting P-type ZnO.

Thus, the present proposal aims to study the mechanisms of doping in ZnO to optimize the conditions for synthesis of ZnO thin film types P.Will be on the effect of temperature, time annealing and the lithium concentration on the electrical properties of these layers. The aim is to find the parameters that need to act to increase the electrical conductivity of p-type ZnO is the major technological barrier to the development of this sector.

The effects of Li content on the crystallinity, morphological and optical properties of ZnO films were assessed by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM). XRD patterns of the films showed the hexagonal wurtzite type polycrystalline structure. The SEM measurement showed that the surface morphology of the films was affected from the lithium incorporation. The transmittance, refractive index, extinction coefficient and bandgap have been analyzed by optical study .the optimized results obtained at 20 at. % Li-doped concentration.

Poster session 1

Thursday, September 10th, 2015

Time: Afternoon 18.00 – 19.00

Energy and Exergy Analysis of an Integrated Solar Combined Cycle System (ISCCS) in Morocco

Ibtissam El Housni, Sara Mtougui, Lahoucine Bahmad and Abdellah Bah

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Nowadays the Integrated Solar Combined Cycle System (ISCCS) have an important role in efficient power generation especially at desert areas. This paper deals with the energy and exergy analysis of an ISCCS in the Moroccan climatic conditions, using design plant data. We will use the three balance equations, i.e., mass, energy and exergy balance equations to locate the irreversibility, energy and exergy losses of each component of the plant and pinpoint sites of primary exergy destruction. To optimize the ISCCS we will do an exergo-economic analysis.

Nanostructures for Organic Solar Cells from Anodized Aluminum Templates

A.J. Goszczak, J. Adam, P. Cielecki, J. Fiutowski, H-G Rubahn and M. Madsen

Increasing the efficiency of Organic Solar Cells (OSC) by implementation of metal nanostructures currently is and has for the past few years been of high interest. In this context, the present work focuses on efficiency enhancement of OSC by structuring the electrodes at the nanoscale. This is done with the use of metal nanostructures via a rapid fabrication method, combined with nano-imprinting techniques. More specifically nanostructures have been fabricated using a porous template made by anodization of Aluminum.

Al possesses the intriguing property that by anodizing it under specific conditions one can obtain a porous anodic alumina (PAA) template. Such templates are fast to fabricate and scalable to industrial production level. Here PAA templates have been fabricated by anodizing a submicron evaporated Al layer on supported surfaces in three different electrolyte solutions, sulfuric, oxalic and phosphoric acid. Controlling of the anodization conditions leads to control of the dimensions of the pores in the PAA templates.

The formation mechanism of the porous templates leads automatically to the nanopatterning of the underlying Al surface, which is covered with nanoscale Al dimples. Here we demonstrate that such non-periodic metallic surfaces present field-enhancement effects, which here is investigated by subjecting the nanoscale dimple structures to a laser ablation technique, by covering the freshly fabricated Al dimple templates with a thin layer of PMMA and exposing it to femtosecond laser pulses. FDTD simulations were performed to observe the correlation with the experimental part.

Moreover the Al dimples have been used for fabrication of nanopatterned electrode surfaces. This has been done by fabrication of a soft mold from the Al dimples, followed by a nanoimprinting process step, which provides a nanostructured surface for OSC devices. All the samples in the different fabrication steps were characterized by SEM and AFM to obtain details of the morphology of the structures.

Simulating the Feasibility of Installing a Smart Grid in Rabat, Morocco

Sara Mtougui, Ibtissam El Housni, Lahoucine Bahmad and Abdellah Bah

University Mohammed V, Faculty of Sciences Av. Ibn Batouta, B.P. 1014, Rabat, Morocco

In the last decade smart grids are more and more increasing in the world. It's a new strategy for demand response of electricity energy needs. Unfortunately, here in Morocco there is no grid-connected PV that's why we study the feasibility of installing a smart grid in Rabat, Morocco. Our study is based on NASA's data and software of sizing PV installation as HOMER, Retscreen, PVSyst to evaluate three aspects of installation, the technical, economical and environmental one. This study aims to facilitate the task and to encourage citizens to use green energy.

Use Electro-Actifs Polymers in the Energy Harvesting Application to TTU

Chakhchaoui N. [1,2], Ennamiri H.[2], Eddiai A.[3] and Boughaleb Y.[1, 4]

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The advances in low power electronics, wireless technology, and wearable computing devices have led to an ever increasing amount of electronics carried by a person. While these devices increase our ability to communicate they can also be cumbersome and require the use of electrochemical batteries to supply power to each device. In the case of emergency personnel, field-based environmental researchers, or backcountry sport enthusiasts, these devices also result in substantial loads. These loads are further increased due to the need to carry heavy electrochemical batteries as the energy source for each device, greatly increasing the carried load.

The objective of this work is to develop a toggle rolling Textile with the developed composite (based on synthetic composite PU), which can generate electrical energy from the differential forces. The purpose of this system is to make transparent energy recovery device for the user as well as endurance and dexterity is not compromised. Electromechanical Characterization and Evaluation of the performance of these polymers for energy recovery. This paper will develop a theoretical model of the piezoelectric loop and perform experimental tests to validate the performance of the crop of model accuracy and energy.

Effect of Different Signals of Polarization Using Electrostrictive Polymers for Harvesting Energy

Z. Sabri[1], A. Eddiai[1], M. Meddad[2], M. Mazroui[1] and M. Rguiti[3]

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Electrostrictive materials can be employed to convert the mechanical energy, such as ambient vibration in electric energy or in a large number of areas such as artificial muscles or vibration control. The aim of this work consists in studying the effects of different signals of polarization of electric field in order to develop a more in-depth understanding of the changes in system response for increased the harvested power. In fact, the theory is detailed then, with the three signals by applying amplitude of electric field of 10 MV/m and transverse strain of 3% and considering a phase shift between them in order to maximize the energy density. The simulation results are compared with experimental ones and good agreements are found.

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3D Graphene-Based Material as Catalyst Support Material for Fuel Cells

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Porous three-dimensional graphene based carbon nanostructures was prepared via in-situ hydrothermal polymerization and carbonization followed by chemical activation and graphitization. In this process, which was initially developed for preparation of electrode materials for supercapacitors [1], an aqueous suspension of hummers graphite oxide was mixed with an organic precursor and heated in a sealed Teflon lined autoclave at 180 °C for 12 hours. The resulting product was washed with ultrapure water and dried in vacuum. Then it was mixed and ground together with potassium hydroxide and activated in a tube furnace in an argon atmosphere at temperature in the range of 800-900 °C. After activation the material was washed with a dilute hydrochloride solution followed by ultrapure water until a pH value of 7 was achieved. Finally the now activated carbon material was dried in vacuum.

Platinum nanoparticles were then precipitated on the surface of the synthesized carbon materials using a modified polyol method to create catalyst materials for fuel cells. The catalytic properties of these platinum coated three-dimensional graphene based carbon nanostructures with regards to hydrogen oxidation, oxygen reduction and methanol oxidation were then characterized using cyclic voltammetric techniques.

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Temperature Influence on Microstructure and Optical Properties of TiO_2-Au Monolayer Thin Films

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TiO_2-Au-nanocomposite thin films were successfully deposited on quartz substrate using sol-gel technique. The influence of the annealing temperature on microstructure and optical properties was examined. SEM micrographs showed homogeneous distribution of Au nanoparticles when annealing temperature increased. X-ray diffraction and Raman spectroscopy allowed the identification of only the anatase phase formation at 500 °C that persisted up to 800 °C. Optical spectra showed the presence of localized plasmonic resonance from Au nanoparticles that red-shifted with increasing annealing temperature (larger Au-particle size). The effective medium model was used to describe the spectrophotometric measurements. Numerical calculations have led to the determination of optical constants. Using common the oretical models we have determined the Cauchy parameters of the refractive index. The band gap E_g of TiO_2-Au thin films was found to decrease from 3.21 to 2.71 eV with increasing temperature. The refractive index behavior is adequately described by the single oscillator model proposed by Wemple and DiDomenico whereby the oscillator parameters values were determined.

Investigation of the Structural, Microstructural and Optical Properties of Titanate Strontium $SrTiO_3$

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The investigation of the structural properties of titanate strontium $SrTiO_3$ (ST) was carried out. The microstructure, the morphologie and the composition of the synthesized samples were investigated by X-ray diffraction (XRD), AES, IR and Raman spectroscopy. A fitting software was used to adjust the Raman spectra to analyzed the influence of temperature samples on the Raman frequencies and on the full width at half-maximum (FWHM) of peaks of the ST Raman spectra. The results of Raman spectroscopy showed that the 443cm^{-1} mode is most affected by temperature, followed by the mode located at 613cm^{-1}. Furthermore, the width at half maxima of all modes increases with the increase in the temperature. Their optical properties were investigated by ultraviolet visible (UV-vis) absorption and photoluminescence (PL) measurements. UV-vis absorption measurements revealed the optical band gap (Egap) value of this material using the Kubelka–Munk equation based on the transformation of diffuse reflectance measurements to estimate Egap values with good accuracy.

The Relaxation and the Diffusion of Au and Pt Adatoms on Missing Row Reconstructed Surfaces of Gold

H.Gounaya[1], E. El Koraychy[1], K. Sbiaai[2,3], M. Mazroui[1] and Y. Boughaleb[1,3]

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Adatoms diffusion on metal surfaces has been attracted a considerable interest of physics community because of the potential applications in several fields such asin electronic devices (nanotechnology), chemical reactions, catalysis and micro-semiconductors.

In this work, we investigated the adsorption and the diffusion of Au and Pt adatoms on the unreconstructed (1×1) and reconstructed (1×2) (1×3) and (1×4) Au (110) surfaces for homogenous Au/Au and heterogeneous Pt/Au systems by using quenched molecular dynamics simulation combined with the interatomic potential described by the embedded atom method. The multilayer and adatom relaxations were calculated and compared with available theoretical results and a good agreement was obtained. On the other side, the static energy barrier for hopping diffusion and the adsorption energy were calculated for the ideal (1×1) and (1×2) (1×3) and (1×4) missing row reconstructed geometries.

Thermal Effects on I-V Characteristics for GaAs MESFET Devices

C.Kaddour[1], C.Azizi[2], S.Khemissi and M.Zaabat

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Abstract -Thermal effects in electronic devices are studied to investigate their influence on reliability and electrical performance. In this study, we present a temperature dependent analytical model for GaAs MESFET .The model is based on the electron mobility and saturation velocity and it is further extended to predict the temperature dependence of drain conductance and transconductance. The results of this work present the properties of the component with different temperatures.

Structural Characterization and Superconducting Properties of Nb_3Al by Combustion Synthesis

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In this work we present, the synthesis of superconductive intermetallic compound, of crystallographic structure of type A15 (Nb_3Al) presenting a critical temperature of 18°K. The preparation of mixtures was crushed dry in one steel jar by means of a global crusher in a weak speed of 150Tr／m. Powder her Nb_3Al is compacted under cold conditions united uniaxially in a press (12 tons), pressure of P=2000Psi. By using the electrothermal explosion (ETE) initiated by the heavy current (400 A), the obtained samples were characterized of the phase composition by the diffraction technique of the X-rays. Further studies have been carried out by field emission scanning electron (FESEM) and optical microscopy. The energy-dispersive X-rays microanalysis (EDX) and Auger spectroscopy was used to determine the phase composition of the phase formation.

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Encapsulation of Gold Nanoparticles onto Green Tea Extracts-Modified Chitosan Flakes as Catalyst for 4-Nitrophenol Reduction

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In this study, phenolic compound extracted from natural green tea was encapsulated onto chitosan (CS) flakes by the aid of plasma in liquid phase. An important component in green tea is epigallocatechin gallate (EGCG) which has good structure for forming a stable five-membered chelating ring with gold ions (Au^{3+}). So that, the chelated Au^{3+} ions can be reduced to gold nanoparticles (AuNPs) while the EGCG is oxidized into quinone compounds. Due to this nature, when the EGCG is encapsulated onto the CS flakes, the AuNPs can be deposited on the EGCG-modified CS when the flakes are immersed in gold precursor solution. In order to improve the encapsulation efficiency, we generated plasma in the green tea solution containing CS flakes during the encapsulation. Effect of the plasma conditions on the formation of AuNPs was studied. Results showed that color of the CS flakes changed from white to light brown after they were modified with green tea. They were then changed to red brown when the flakes were immersed in gold precursor ($HAuCl_4$) aqueous solution, suggesting that the AuNPs were syntesized and deposited on the CS surface. TEM images revealed that the AuNPs distributed evenly on the CS. These EGCG-modified CS was found to be an active inorganic-organic hybrid catalyst for the reduction of 4-nitrophenol to 4-aminophenol. They can

also be easily recovered and reused because of the strong affinity between AuNP and CS surface.

Fig. 1 Chitosan flakes before and after modified with green tea extracts and deposited with AuNPs

PH Effect on the Synthesis of Cu_2O/CuO Nanoparticles by Sol-Gel Method in a Glycolic Medium

Najoua Zayyoun[1], Larbi Laânab[1] and Jaber Boujemaa[2]

[1]LCS, Faculty of Sciences. Mohammed V University, Rabat, Morocco
[2]UATRS,BP.8027 Nations Unies,10102 Rabat, Morocco

The cuprous oxide and cupric oxide are attracting increasing attention on account of their potential applications and unique properties. CuO and Cu_2O nanoparticles find application in the field of catalysis, sensors, and as an electrode in Li-ion batteries. However, synthetically it is challenging to prepare these oxides in pure phases. Especially the synthesis of Cu_2O without any impurities is regarded as a hard task due to the better stability of copper in +2 state as compared to +1 state.

In this paper, we report the controlled synthesis of Cu_2O and CuO from the same precursor by Sol-Gel method using the pH of the solution as the only variable parameter. XRD results confirmed the formation of pure CuO with a monoclinic structure at higher pH, whereas the pure Cu_2O was formed at lower pH with a cubic structure. TEM image indicates that the as-formed CuO Nps in basic pH are spherical in shape and their size is found to be in the range 5–7 nm. SEM images reveal that the as-obtained Cu_2O Nps in acid pH are cubical and agglomerated into large particles of spherical shapes having a diameter at about 350 ± 50 nm. The gap energy Eg measured by UV–visible spectroscopy of Cu_2O and CuO Nps are 2.2 eV and 4.25 eV respectively.

Preparation and Catalytic Evaluation of Natural Leaf Supported Gold Nanoparticles

Shuhei Yoshida[1], Anyarat Watthanaphanit[1,3] and Nagahiro Saito[1,2,3,4]

[1]Department of Materials, Physics and Energy Engineering, Graduate School of Engineering, Nagoya University, Japan
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[4]JST-CREST, Japan

Nanoparticles have been deposited onto the surface of various supporting materials to enhance their stability and catalytic activity. Owing to the fact that biological systems in nature have solved the problem of designing and synthesizing functional materials with smart nanostructures through the evolution over millions of years, herein, we utilize the natural leaf frame as a template for the deposition of gold nanoparticles (AuNPs). The AuNPs were produced by applying the plasma into gold (III) chloride hydrate aqueous solution where the pieces of leaf frames were distributed in. Effect of the plasma discharge time on the appearance of the deposited AuNPs and the catalytic reduction ability of 4-nitrophenol to 4-aminophenolof the hybrid samples were evaluated. Results revealed that, as the processing time was increased, the peak of 4-nitrophenol decreased and the peak of 4-animophenol increased which should be caused by the increase amount of AuNPs when the plasma discharge time was prolonged. Reusability of the hybrid samples was additionally evaluated. This study suggests the promotion of utilizing natural resources to prepare reusable hybrid inorganic–organic materials to facilitate the reaction for product isolation.

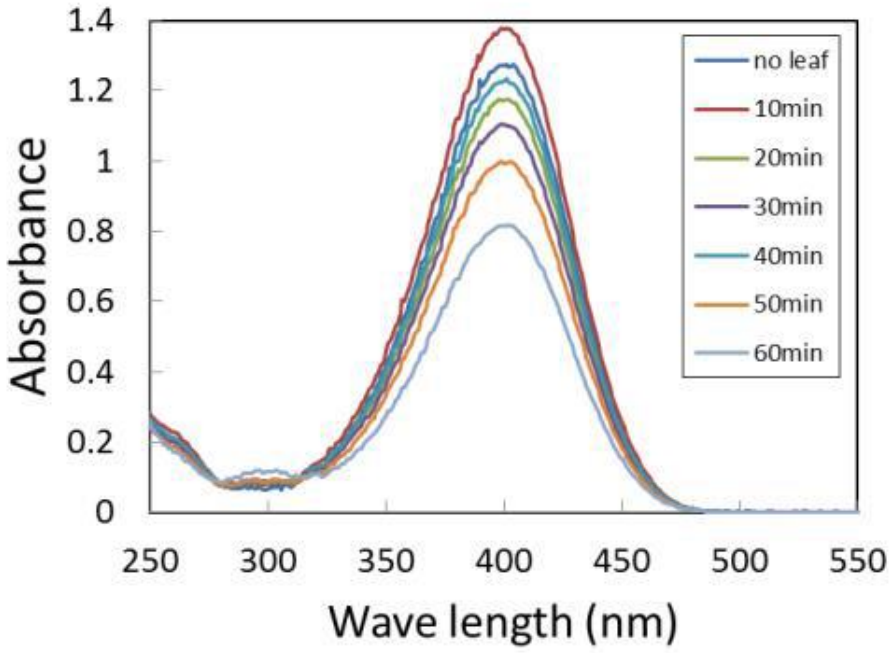

Fig. 1 Reaction profile of 4-nitrophenol to 4-aminophenolusing natural leaf supported gold nanoparticles fabricated from plasma discharge in solution with different discharge times.

Simple One-Step Synthesis of Nanostructured MnO_2Colloidal Suspension by Plasma Discharge in Liquid

Hyemin Kim[1,3], Anyarat Watthanaphanit[1,2] and Nagahiro Saito[1,2,3,4,5]

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[2]Social Innovation Design Center, Institution of Innovation for Future Society, Nagoya University, Japan
[3]Green Mobility Collaborative Research Center, Nagoya University, Japan
[4]EcoTopia Science Institute, Nagoya University, Japan
[5]Japan Science and Technology Agency (JST)–CREST, Japan

Nanoscale transition metal oxide materials have been receiving much attention in scientific and technological fields due to their unique physical and chemical properties. Among them, nanostructured manganese dioxide (MnO_2) is one of the most promising metal oxide owing to its excellent electrochemical properties which lead to multiple applications (i.e. electrode material for energy storage system, oxidative degradation substance, catalyst, biosensor, magnetic material and ion-exchanger, etc.) as well as its low cost, abundance, and eco-friendliness [1–2]. Avariety of synthesis techniques have therefore been exploited to obtain the nanostructured MnO_2, especially in its colloidal form [3]. In this study, colloidal MnO_2 was successfully synthesized by discharging the plasma in potassium permanganate ($KMnO_4$) aqueous solution in the absence of any additional reagents and templates. To understand the reduction mechanism of MnO_4 –to MnO_2 in the system, chemical compositions of the samples were measured by optical emission spectrometer (OES) during the plasma generation. The presence of reactive hydrogen species is responsible for the reduction of permanganate ion (MnO_4–) to manganese dioxide (MnO_2). MnO_2 formation was also confirmed by ultraviolet-visible spectroscopy (UV-vis)

according to the time-course at 2 minutes interval. After the plasma was generated, the absorption peaks in the range of 500–570 nm corresponding to MnO_4–gradually disappeared while a new absorption peak at around 360 nm assigning to MnO_2 nanostructures emerged. It could be clearly seen that solution color was changed from purple to brown when the discharge time was prolonged. The colloidal suspension of the as-prepared MnO_2 exhibited good stability over 6 month which was additionally confirmed by zeta-potential analysis. Morphology and structure of the nanostructured MnO_2 were analyzed by transmission electron microscope (TEM), energy dispersive X-ray spectrometry (EDS) element mapping and Fourier transform infrared spectroscopy (FT-IR).

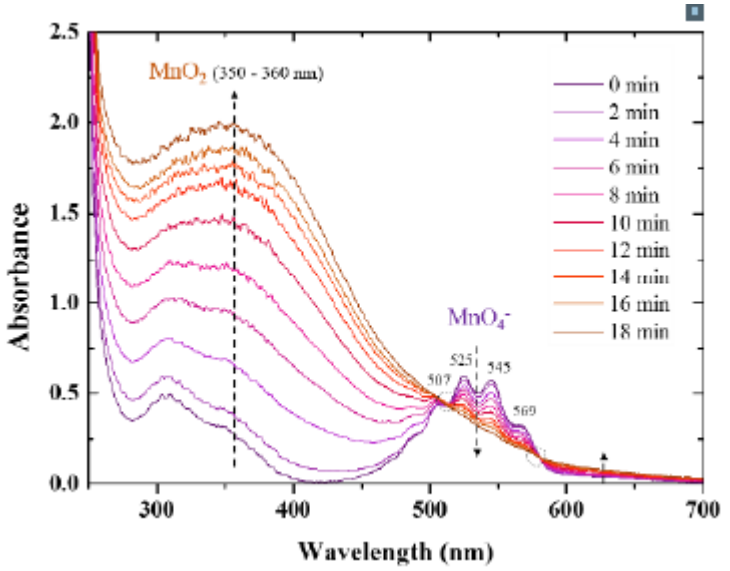

Fig.1 UV-vis absorption spectra of colloidal MnO_2 nanostructures by discharging time

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Synthesis of Black Titania Spheres with Efficient Visible-Light Photocatalytic Activity by Water Plasma

Gasidit Panomsuwan[1], Anyarat Watthanaphanit[2,3], Takahiro Ishizakiae[1,5] and Nagahiro Saito [2,3,4,5]

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[2]Social Innovation Design Center (SIDC), Institute of Innovation for Future Society, Nagoya University, Nagoya, Japan
[3]Department of Materials, Physics and Energy Engineering, Graduate School of Engineering, Nagoya University, Nagoya, Japan
[4]Green Mobility Collaborative Research Center, Nagoya University, Nagoya, Japan
[5] Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency (JST), Saitama, Japan

A green method assisted by water plasma has been developed for the synthesis of stable-black titania (H-TiO_{2-x}) spheres at a low temperature and atmospheric pressure. The *in situ* production of highly energetic OH and H species from water plasma play an essential role in the oxidation and hydrogenation reactions of the H-TiO_{2-x} spheres. The visible-light photocatalytic activity of the H-TiO_{2-x} sphere was studied via degradation of methylene blue (MB) dye. Results revealed that important factors leading to the promotion of photocatalytic activity of the H-TiO_{2-x} were the spheres' large accessible surface areas, visible-light absorptions, and defect sites (i.e., oxygen vacancies and Ti^{3+} ions). We believe that this synthetic route can potentially be extended to the design and synthesis of various defective metal-oxide particles for advanced photocatalysis and energy storage/conversion applications.

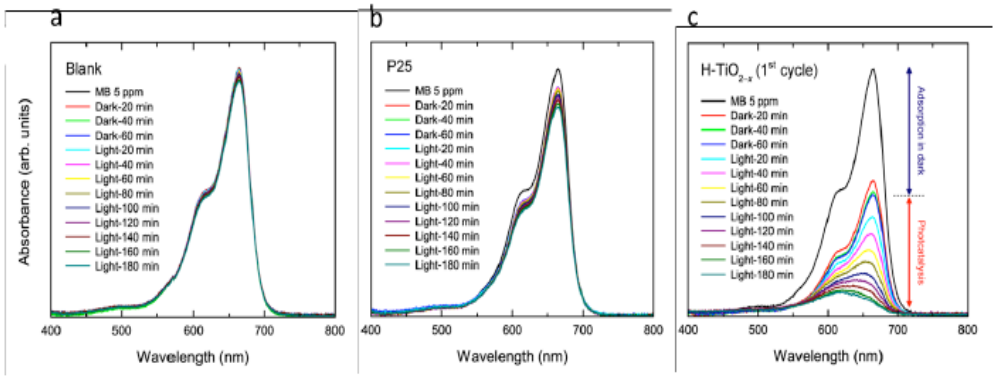

Fig. 1 UV-visible absorption spectra of MB solution at different irradiation times: (a) without photocatalyst, (b) P25 (control), and (c) H-TiO $_{2-x}$ (1st cycle)

Photocatalytic Degradation of Methylorange by TiO_2 Nanostructured Thin Film

Sana El-Kacemi[1,2] , Mohamed Hamdani[1] and Mohammed Es-Souni[2]

[1]Laboratoire de chimie physique, Faculté des sciences, Université Ibn Zohr, BP 8106, Cité Dakhla, Agadir, Maroc
[2]Institut de technologie de surface, Université des sciences appliquées, Grenzstrasse 3, 24149 Kiel, Allemagne

Currently, the research activity in the field of photodegradation of wastewater is considerably amplified. This interest is mainly due to problems of pollution and stricter safety regulations adopted by several countries in many industrial sectors. Hence the need to develop new materials, more sensitive and selective, to degrade organic pollutants present in these waters.

This work fits into the general framework of the development of a new process for physico-chemical treatment (photochemical) for environmental protection. It concerns to highlight the new nanostructured oxide materials for use in the treatment of polluted water. In our study we are interested in the implementation of titanium dioxide thin films and to study the photocatalytic properties.

The TiO_2 thin films were deposited on substrates of graphite felt by immersion followed by calcination at different temperatures. Different samples were prepared and characterized by X-ray diffraction, scanning electron microscopy (SEM) and Raman spectroscopy.

The photocatalytic properties of TiO_2 thin films on molecules of methyl orange have been studied.

Synthesis of Nickel Nanoparticles in Aqueous Copolymer Emulsion

A. Moumen[1], W. Halim[1], K. Abderrafii[2] and S. Ouaskit[1]

[1]Laboratoire de la Physique de la Matière Condensée (URAC10), Faculté des Sciences Ben M'sik, Université Hassan II Casablanca, Maroc
[2]Institut de Microelectronica de Madrid (IMM) Isaac Newton 28760 tres cantos madrid, Spain

In this study, Nickel nanoparticles were prepared by polyol process under different concentration of latex copolymers. This method has been realized by mixture solution containing precursor of Nickel, (NaOH) as catalysis, ethylene glycol as solvent and a reducing agent and latex copolymer as reducing and stabilizing agents. The obtained nanoparticles were characterized by IR spectroscopy, X-Ray diffraction and the transmission electron microscopy, and we have demonstrated the crucial effect of latex copolymers and amount of NaOH in assembling of Nickel nanoparticles. The dominate shape is a sphere nanoparticles with an uniform distribution sizes of 2- 6 nm and a small amounts of single crystalline gold nanorods. The formation mechanism of Nickel nanostructures was discussed.

Absorption of Visible Light by GaAs and GaN Nanosheet

M. Houmad[1], O. Dakir[1], A. Benyoussef[1,2,3] and A. El Kenz[1,*]

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[2]Institute for Nanomaterials and Nanotechnology, MASCIR (Moroccan Fondation for Advanced Science, Innovation and Research), Rabat, Morocco
[3]Hassan II Academy of Science and Technology Rabat Morocco

In this work we study the electronic and optical properties of GaAs and GaN nanosheet (2D monolayer) using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method with the Generalized Gradient Approximation (GGA) within wien2k package. The dielectric tensor is derived within the random phase approximation (RPA). We compared the electronic structure and the optical properties between GaAs and GaN nanosheet such as the dielectric function, reflectivity, absorption coefficient and optical conductivity which are calculated for both perpendicular and parallel electric field polarizations. We show that GaN and GaAs nanosheet have a direct band gap. The reflectivity of GaN nanosheet is lower than that of GaAs nanosheet. Finally, we show that the absorption coefficient of GaAs nanosheet is higher than that of GaN nanosheet.

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Morning sessions

Friday, September 11th, 2015

Plenary session

Time: 8.30 – 9.15

Room: Lecture hall 1

Chair: Aline Rougier

Friday, 2015-09-11	08.30	Plenary talk	Plenary talks	Lecture hall 1

Ultrafast Dynamics in Metal-Organic-Frameworks (MOFs)

M. Gutierrez[1], F. Sanchez[2] and A. Douhal[1]

[1]Departamento de Química Física, Facultad de Ciencias Ambientales y Bioquímica, INAMOL, Campus Tecnólogico de Toledo. Avenida Carlos III, S/N, Universidad de Castilla-La Mancha (UCLM), 45071, Toledo, Spain
[2]Instituto de Química Orgánica, CSIC, Juan de la Cievra, 3, 28006 Madrid, Spain

Metal-Organic Framework (MOF) materials have aroused a great interest in the scientific community owing to their excellent structural properties like high specific surface areas, large pore volumes as well as their free and accessible cavities [1]. MOF has been then recently employed in different fields of science and technology like optoelectronic devices [2], fluorescent sensors [3], and drug photodelivery [4]. Exploring the spectroscopy and photodynamics properties of MOFs is thus fundamental to a better understanding and use.

In this talk, I will show and discuss our recent results on using femto-nanosecond time-resolved emission techniques to interrogate the photodynamics of a Zr-based MOF in suspensions, and in solid-state. The experiments indicate a strong interaction between neighbouring ligands giving excimers formation in all the studied suspensions. I will also show and discuss the origin of the tunable emission and photodynamics of the same MOF containing fluorescent organic dyes, and possible applications in sensing and optoelectronical devices.

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[4] di Nunzio, M. R.; Agostoni, V.; Cohen, B.; Gref, R.; Douhal, A. *J. Med. Chem.* 2013, *57* (2), 411-420.

Acknowledgement: This work was supported by MINECO through projects MAT2011-25472, Consolider Ingenio 2010 (CSD2009-0050, MULTICAT), and PRI-PIBIN-2011-1283. M.G thanks the MINECO for the FPI fellowship

Energy Materials

Time: 10.20 – 12.30

Room: Lecture hall 2

Chair: Nagahiro Saito

Friday, 2015-09-11	10.20	Invited talk	Energy materials	Lecture hall 2

Stereolithographic Additive Manufacturing of Ceramics Dendrites with Geometric Fluctuations for Energy and Material Flows Modulation

Soshu Kirihara

Joining and Welding Research Institute, Osaka University

Ceramics dendrites with spatially ordered micro cavities were successfully fabricated by three dimensional printing of stereolithography. Micro lattices pattern were propagated spatially in computer graphic space. Ceramics nanoparticles were dispersed in to photo sensitive liquid resins to obtain thixotropic slurries. The paste material was spread on a grass substrate by using a mechanical knife edge, and an ultra violet laser beam was scanned on the surface to create cross sectional solid layer. The ceramics dendrites were obtained by layer stacking. The composite precursor was dewaxed and sintered in an air atmosphere. Through this process, solid electrolyte dendrites of yttria stabilized zirconia were fabricated for fuel cell miniaturizations Gaseous fluid profiles and pressure distributions in the formed ceramic lattices were visualized and analyzed by a finite element method. Subsequently, alumina photonic crystals with a diamond lattice structure were fabricated. Electromagnetic wave properties were measured by using a terahertz time domain spectroscopy. A complete photonic band gap was exhibited, and a localized mode to select the wavelength was obtained by introducing a defect cavity. Moreover, artificial bones of hydroxyapatite scaffolds were modeled to realize excellent biological compatibilities. Graded porous structures in the artificial bones were processed.

Enhancement of Photoluminescence and Electrochemical Activity in Porous Silicon/Metal Oxide Composite Materials

Minoru Mizuhata

Department of Chemical Science and Engineering, Graduate School of Engineering, Kobe University, 1-1 Rokkodai-cho, Nada, Kobe (Japan)

Porous silicon (PSi) is fabricated by anodic oxidation of Si wafer in HF/organic solvent solution. Pore size is controlled by resistivity of Si wafer and reaction condition. We have fabricated various oxide and sulphide composite with porous silicon; such as CeO_2/PSi, TiO_2/PSi, and ZnS/PSi. In general, the chemical reaction in an aqueous solution is suitable to deposit thin film among complex structured substrate because of its short mean free path of reactive species. In this leture, we introduce the fabrication of these thin films deposited on the surface of pores in porous silicon without the plugging of pores by electrodeposition. In this abstract, ZnS system is written.

PSi was fabricated by the anodization of n-Si (100) wafer in HF/EtOH/H_2O solution under galvanostatic conditionn. Pore diameter was 20-80 nm and pore depth was 8-50 μm. Pore size was controlled by HF concentration and etching time. ZnS was deposited under galvanostatic condition (0.44-8.85 mA/cm^2) in the aqueous solution which contains $ZnSO_4$, $Na_2S_2O_3$, and glycerol.

ZnS was deposited on PSi whose pore diameter was 80 nm at various current densities as shown in Fig. 1. At high current density deposited ZnS plugged the pore, whereas at low current density, ZnS was deposited among the pore wall without plugging the pore. Zn and S were distributed over the pore wall at low current density. When a high electric current applied to a porous electrode, the electric field has been concentrated at the openings of pores and the electric field spread out in the pores at the low electric current. The PL spectra due to the ZnS/PSi composites s had two peaks at 430 (blue) and 530 nm (green). The PL intensity was decreased with an increase of current density, hence PL intensity was decreased in the case of high current density, it is thought (1) reduction of ZnS to metal Zn and (2) segregation of ZnS on theupper of the pore as reasons. The expansion of surface area lead to enhancement of PL intensity. Deposit amount of Zn was increased with deposition time linearly, whereas the PL intensity was increased not linearly as shown in Fig. 2, thus an increase of PL intensity resulted from not only an increase of deposit amount of Zn.

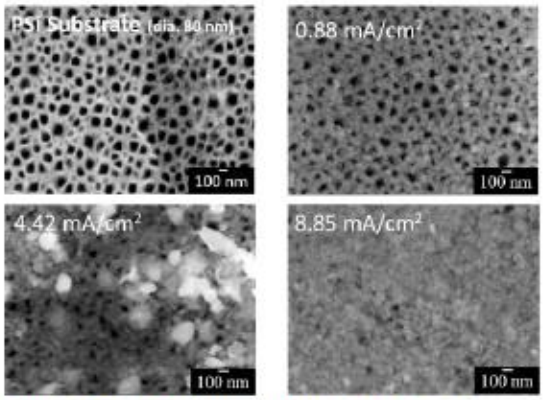

Fig. 1 SEM images of PSi substrate and ZnS/PSi composites deposited at various current density for 60 min.

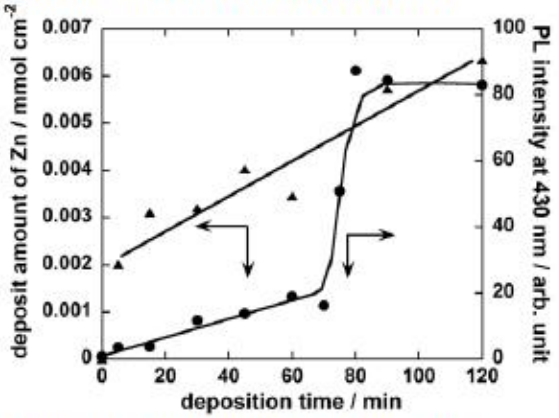

Fig. 2 Deposit amount of Zn and PL intensity at various deposition times.

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Alloying and Size Effects on the Sorption Properties of Mg-Based Hydrides

Fermin Cuevas, Claudia Zlotea, Junxian Zhang and Michel Latroche

Institut de Chimie et des Matériaux Paris-Est, CNRS-UPEC UMR 7182, 2-8, rue Henri Dunant, 94320 Thiais, France

Magnesium, a cheap and abundant element, has been extensively studied as a hydrogen store because of its high specific capacity (7.7 wt.% H). Moreover, magnesium forms a reversible hydride but its high thermodynamic stability (enthalpy of decomposition 75 kJ/mol H_2 [1]) ant the slow kinetics of the hydrogen sorption reaction makes it poorly efficient for practical hydrogen storage.

Several approaches have been foreseen to improve or tune the sorption properties of this element. Addition of catalysts or alloying with transition metals has been proposed [2] and leads to significant enhancement of the hydrogenation properties. Furthermore, downsizing the particle size allows to significantly increase the solid-gas interface and to decrease the hydrogen diffusion path within the grains.

In the present work, several cases will be presented. Firstly, preparation of complex Mg-based hydrides by reactive ball milling will be considered and their sorption properties will be reported [3-5]. Secondly, the preparation of small Mg_2MH_x (M = transition metals) nanoparticles synthesized into the mesopores of different carbons hosts by wet chemistry method will be described. Such Mg_2MH_y nanoparticles are extremely stable against coalescence during hydrogen sorption cycling and exposure to high temperature. Their properties will be compared to those of pure Mg and MgH_2 nanoparticles [6, 7].

This study opens new routes for successful development of complex hydrides with a better understanding of the underlying nanochemistry.

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Friday, 2015-09-11	11.50	Talk	Energy materials	Lecture hall 2

An In-Depth Study of the Effect of Transition Metals on the Hydrogen Storage Proprieties of MgH_2

M. El Khatabi[1], M. Bhihi[1], M. Lakhal[1], S. Naji[1, 2], H. Labrim[3], A. Benyoussef[1, 4, 5], A. El Kenz[1] and M. Loulidi[1]

[1]LMPHE, (URAC), Faculté des Sciences, Université Mohammed V-Agdal, Rabat, Morocco
[2]Department of Physics, Faculty of Science, Ibb University, Ibb, Yemen
[3]Centre National de l'Energie, des Sciences et des Techniques Nucléaires, Rabat, Morocco
[4]Institute of Nanomaterials and Nanotechnology, MAScIR, Rabat, Morocco
[5]Hassan II Academy of Science and Technology, Rabat, Morocco

We propose a DFT study, to understand the improvement of hydrogen storage proprieties, of MgH_2 doped with different transition metals TM= Sc, Ti, V, Cr, Y, Zr, Nb, Mo. The TMs are either from the same group or the same period. The calculations were conducted by all-electron full-potential local-orbital minimum-basis scheme (FPLO9.00-34). Based on our results we observed a reduction of the heat of formation ΔH and also of the desorption temperature T_d. Nb appears to be the best substitution element, with an ideal heat of formation that equals 40.96 kJ/mol. A detailed study of the effect of each TM on the stability of MgH_2 was carried on. The discussion was based on the TMs electronegativity, the charge exchange between the system elements, and finally the density of states.

Optical and Photocatalytic Properties of $BiVO_4$ Thin Films

R. Mirabal[1,2], O. Depablos-Rivera[1,2], M Thalluri[3], J.-C. Medina-Alvarez[1,2], M. Bizarro[1], J. Perez-Alvarez[1], S. E. Rodil[1,2] and A. Zeinert[4]

[1]Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Mexico City, Mexico
[2]Posgrado en Ciencia e Ingeniería de Materiales, Universidad Nacional Autónoma de México, Mexico City, Mexico
[3]Chemical Engineering (DISAT), Politechnico of Turin, Italy
[4]Laboratoire de Physique de la Matière Condensée, Université de Picardie Jules Verne, 33 rue Saint Leu, 80039 Amiens Cedex 1, France

Monoclinic $BiVO_4$ thin films are considered as an interesting candidate for photoactive materials which could be used for water-splitting as a photoanode or for organic pollutant removal [1, 2].

In this work, we present the structural, optical and photocatalytic properties of $BiVO_4$ thin films produced by a dual magnetron sputtering process using both Bi_2O_3 (a-phase, 99.98% purity) and V (99.9 % purity) targets under and $Ar:O_2$ atmosphere with a ratio of 18:2 respectively for different depositions conditions and post-deposition treatments. The dual process is chosen to better control the Bi/V ratio since Bi and V have very different sputtering yields. In particular, the influence of a chemical treatment using potassium hydroxide (KOH) on the optical properties and different dye discolorations (blue acid, methyl orange) will be discussed. Recently we showed that the KOH treatment can dramatically improve the response for photocurrent in sputtered $BiVO_4$ photoanodes [3].

The optical properties were studied by reflectance and transmittance spectroscopy, where the spectra were fitted to obtain the refractive index

dispersion and the optical band gap of the $BiVO_4$ as a function of the film structure, as determined by X-ray diffraction and Raman spectroscopy.

[1] Le Chen et al., J. Phys. Chem. C, 117, (2013) 21635−21642
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Acknowledgements: Economical support for this work was provided by both BisNano and PHOCSCLEEN projects, The research leading to these results has received funding the European Community Seven Framework Programme (FP7-NMP-2010-EU-MEXICO) and CONACYT under grand agreements N° 263878 and 125141 (BisNano), respectively.

Afternoon sessions

Friday, September 11th, 2015

Plenary session

Time: 14.00 – 14.45

Room: Lecture hall 1

Chair: Horst-Günther Rubahn

Recombination Pathways in High Efficiency Organic Solar Cells

Vladimir Dyakonov

Chair of Experimental Physics VI, Institute of Physics, Julius-Maximilian University of Würzburg, Am Hubland, 97074 Würzburg, Germany

To increase the power conversion efficiency of organic solar cells it would be extremely advantageous to improve harvesting of singlet, triplet and charge transfer excitons as well as to suppress recombination. We analyse the limitations of solar cell performance of devices based on poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2- b:4,5-b']dithiophene-2,6-diyl] [3-fluoro-2-[(2- ethylhexyl)carbonyl] thieno [3,4-b] thiophenediyl]] (PTB7):[6,6]-phenyl-C71-butyric acid (PC71BM) bulk heterojunctions. The dramatic change of the power conversion efficiency from about 3% to above 7% upon adding a co-solvent is observed. [1] Using a combination of various transient photoconductivity techniques, we study the influence of nongeminate and geminate recombination losses and discuss them in view of Langevin and trapassisted recombination. Further, by means of spin sensitive techniques, we show that electron back transfer from charge transfer to triplet state takes place and can be responsible for the reduced solar cell performance, too. A decay of charge transfer states into free charge carriers or, alternatively, electron back transfer reactions is shown to depend on the energy levels of constituting donor and acceptor molecules [2] and on the morphology of blends [3].

[1] Nongeminate and Geminate Recombination in PTB7:PC71BM solar cells. A. Förtig, J. Kniepert, M. Glücker, V. Dyakonov, D. Neher, C. Deibel, Adv. Funct. Mater. 24, 1306 (2014).
[2] Triplet exciton generation in bulk-heterojunction solar cells based on endohedral fullerenes. M. Liedtke, A. Sperlich, H. Kraus, A. Baumann, C. Deibel, M. Wirix, J. Loos, C. Cardona, V. Dyakonov, J. Am. Chem. Soc. 133, 9088 (2011).
[3] Morphology Dependent Triplet Exciton Loss Pathway in PTB7:PC71BM Blend Films. H. Kraus, M. C. Heiber, S. Väth, J. Kern, C. Deibel, A. Sperlich, V. Dyakonov (submitted).

Organic Solar Cells

Time: 14.50 – 16.20

Room: Seminar room 1

Chair: Malle Krunks

Friday, 2015-09-11	14.50	Invited talk	Organic solar cells	Seminar room 1

Modeling Nanostructure-Enhanced Light Trapping in Organic Solar Cells

Jost Adam

NanoSyd, Mads Clausen Institute, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark

A promising approach for improving the power conversion efficiencies of organic solar cells (OSCs) is by incorporating nanostructures in their thin film architecture to improve the light absorption in the device's active polymer layers. Here, we present a modelling framework for the prediction of optical and plasmonic field enhancement by nanostructures in (or close to) the active layers and electrodes in OSCs. We incorporate finite-difference time-domain (FDTD) calculations alongside semi-analytical approaches, as the rigorous coupled-wave analysis (RCWA) and mode-coupling theory. Our simulation results are closely related to and verified by our group's experimental outcomes. We will especially discuss latest results regarding the light trapping by (multi-)periodic [1] and fractal [2] grating structures, and investigate the effect of an alternative, cheap and large-scale production-compatible method for non-periodic electrode structuring by pores of controlled dimensions, formed through anodic oxidation of sputter-deposited high-purity aluminium films [3].

[1] Kluge, C., *et al*. Multi-periodic nanostructures for photon control. *Optics Express*, *22* (S5), A1363. (2014)
[2] Skigin, D., *et al.* Diffraction by fractal metallic supergratings. *Optics Express*, *15*(24), 15628–15636 (2007)
[3] Goszczak, A. J. *et al.* Nanoscale Aluminum dimples for light trapping in organic thin films (submitted)

Friday, 2015-09-11	15.20	Talk	Organic solar cells	Seminar room 1

Stabilization of Organic Solar Cells by Ternary Blending Active Layers with Additives

Vida Turkovic, Sebastian Engmann, Nikos Tsierkezos, Harald Hoppe, Morten Madsen, Horst-Günter Rubahn, Uwe Ritter and Gerhard Gobsch

Vida Engmann, Syddansk Universitet, Mads Clausen Instituttet, NanoSYDm, OPV Group, Alsion 2, 6400 Sønderborg, Denmark

The field of organic photovoltaic has been steadily developing over the past decades, making them competitive with other thin film technologies. Still, although the peak efficiencies reach now over 10%, and the first products have emerged on the market, they are still considered to be an exotic niche product, mostly due to their comparably poor stability.

In our study we investigated a novel way for stability improvement, by ternary blending the active layers with small portions of stabilizing compounds of different classes of antioxidants, radical scavengers and light stabilizers. The compounds are investigated for use in bulk-heterojunction OPV, and miscroscopically and spectroscopically characterized under ISOS-3 conditions with respect to the initial power conversion efficiency and the long-term stability improvement under illumination in ambient conditions. Observed differences in the stabilization of tested additives are discussed in terms of energetic trap states formation within the HOMO/LUMO gap of the photoactive material, morphological changes, and chemical structure.

Friday, 2015-09-11	15.40	Talk	Organic solar cells	Seminar room 1

Organic Solar Cells Integrated in Smart Textile

Hajar Jaouani[1,2],Denoun SaifaouiI[1],Habiba Ennamiri[2] and Youssef Jouane[3]

[1]*University Hassan II, F. S. Ain Chock, Department of Physics Theory, Casablanca, Morocco*
[2]*Higher School of Textile and Clothing Industries, Laboratory REMTEX, Casablanca, Morocco*
[3]*Kochi University of Technology, Japan*

The most common flexible substrates used for flexible solar cells so far have been synthetic polymers such as polyethylene terephthalate (commonly known as PET) and polyethylene naphthalate (PEN) see figure 1 [1]. However, if organic solar cells are to be applied onto clothes and other soft surfaces –some of which come into direct contact with skin they are required to be human-compatible, non-toxic and non-irritable. Among the possible solutions for such a substrate could be silk, who been addressed by the Sun group directed by Professor Baoquan Sun from Soochow University which used "The natural silk fibroin - extracted from silkworm (Bombyx mori) and cocoon that is a smart material that has several promising feature such as: its good biocompatibility, biodegradability, non-irritability, non-toxicity and favorable mechanical properties, and the high optical transmittance (up to 95%) of the film. "In addition, biodegradable and mechanical properties of silk fibroin substrate can be tailored by controlling the manufacturing process, so that they correspond to the desired requirements for an application in Wearable electronic textiles. "

Friday, 2015-09-11	15.40	Talk	Organic solar cells	Seminar room 1

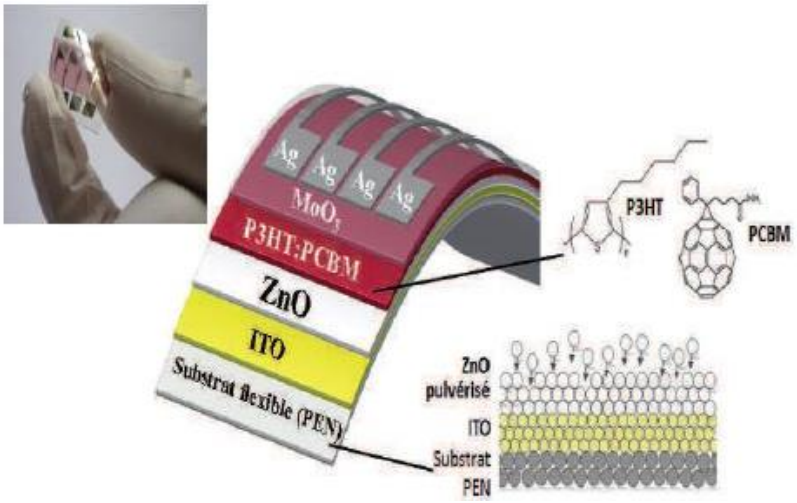


Fig.1 Flexible Organic solar cells by Jouane et Al. [1]

Friday, 2015-09-11	16.00	Talk	Organic solar cells	Seminar room 1

Application of Non-Crystalline MoO_x Films for Optoelectronic Organic Devices

André Luis F. Cauduro[1], Mehrad Ahmadpour[1], Zacarias Eduardo Fabrim[2,4], Paulo Fichtner[2,3], Horst-Günter Rubahn[1] and Morten Madsen[1]

[1]NanoSYD, Mads Clausen Institute, University of Southern Denmark, Alsion 2, 6400 Sønderborg, Denmark
[2]Instituto de Física, Universidade Federal do Rio Grande do Sul (IF-UFRGS), Porto Alegre, Brazil
[3]Department of Metallurgy, Engineering School UFRGS, Porto Alegre, Brazil
[4]PPGMICRO- Graduate program on Microelectronics, Porto Alegre, Brazil

In this work, the effect from applying different oxygen partial pressures ($1.00x10^{-3}$ mbar, $1.20x10^{-3}$ mbar, $1.98x10^{-3}$ mbar and $2.70\ x10^{-3}$ mbar) and different sputtering powers (100 W, 150W, 200 W and 250 W) during the DC sputter deposition of Molybdenum oxide thin-films formed at room temperature were fully investigated. The films were deposited on BK7 glass for analysing the optical transmittance and surface roughness as a function of the deposition parameters. The surface roughness does not change substantially, giving a first indication that the morphology is independent of the oxygen partial pressure in the chamber. The surface roughness was also investigated on commercial ITO substrates, which served as our basis for resistivity measurements using silver top contacts. The films as-deposited with $1.00x10^{-3}$ mbar oxygen partial pressure at 250 W sputtering power were the ones presenting the highest conductivity of around 3.22 S/cm, indicating that although the [O]/[Mo] ratio is low, around 2.57 as extracted from Rutherford Backscattering Spectroscopy (RBS), a semiconducting behaviour is present in the films. As the oxygen concentration increases up to $1.20x10^{-3}$ mbar, a [O]/[Mo] ratio is around 3.00, indicating that a stoichiometric MoO_3 phase is formed. The conductivity of the films at

that oxygen partial pressure decreases by around 5 orders of magnitude to 1.60×10^{-5} S/cm [1].

Since the microstructure of the different films, investigated here from HRTEM, in all cases show amorphous films, the dramatic changes in transmittance and conductivity presented here are not ascribed to different crystal phases in the films, but instead to intrinsic defects, which determine the optical and electrical properties of these films. This work therefore describes an interesting approach for modifying the optical and electrical properties of MoO_x films without employing normally used post-annealing processes, and it therefore presents a more applicable technology for the use of sputtered Molybdenum oxide thin-films in organic electronic and optoelectronic devices, where Molybdenum oxide is widely used as an interfacial layer.
These films are now being exploited as hole extraction layers in novel organic small molecule photovoltaic devices.

[1] Fernandes Cauduro et al. APL **106**, 202101 (2015)

Processing

Time: 14.50 – 16.10

Room: Lecture hall 2

Chair: Soshu Kirihara

Solution Plasma Process for Fine Nanoparticles and Carbon Materials Production

Nagahiro Saito

Department of Materials, Physics and Energy Engineering, Graduate School of Engineering, Nagoya University, Japan Institute of Innovation for Future Society, Nagoya University, Japan Green Mobility Collaborative Research Center, Nagoya University, Japan, Japan Science and Technology Agency (JST) – CREST, Japan

Solution plasma process—a specific type of liquid discharge in solution—is an efficient means of producing fine metal nanoparticles and carbon materials. The process consists of a bipolar power supply which is a power source to generate plasma through electrodes placed in a liquid media. In this reaction field, fine metal nanoparticles can be synthesized by generating plasma in a liquid media containing metal precursors or through sputtering of electrode itself. Mono-, bi- and multi-metallic particles could therefore be synthesized by changing and combining the precursor and electrode of varying types. Novel carbon materials including heteroatom-doped carbon, such as nitrogen-, boron-, and phosphorus-doped carbons can also be produced from aromatic compounds. The heteroatom-doped content is varied by altering the power supply parameters as well as the precursor combinations. These materials with tuned electrical structures work as catalysts for oxygen reduction reaction. The catalyst will be realized as electrode materials for fuel cells and metal-air battery.

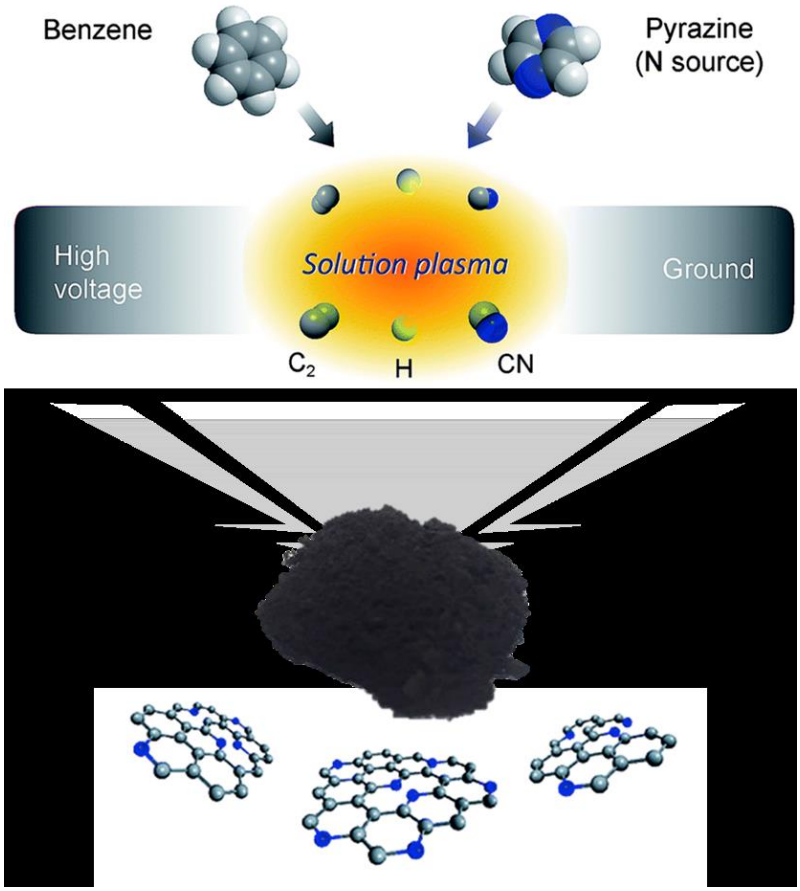


Fig.1 Synthesis of nitrogen-doped carbon by solution plasma process

Macroscopic Optical Antennas with Glassy Disordered Dipolar Composites

Mady Elbahri[1,2,3]

[1]Institute for Materials Science - Nanochemistry and Nanoengineering, CAU-Kiel University Kaiserstr. 2, D-24143 Kiel, Germany
[2]School of Chemical Technology- Nanochemistry and Nanoengineering, Aalto University,
Kemistintie 1, 00076 Aalto, Finland
[3]Helmholtz-Zentrum Geesthacht- Nanochemistry and Nanoengineering, Max-Planck-Str. 1, 21502 Geesthacht, Germany

During the last years, there has been increasing interest in functional nanocomposites due to novel applications ranging from sensors and plasmonics through stretchable electronics and smart coatings to energy conversion and human health. In this context a dipolar composite with a cooperative macroscopic action has not been suggested so far. The present talk aims at introducing a particularly promising new class of functional optical materials based on natural and artificial dipoles embedded in a polymeric/dielectric host where the unique properties arise from the strong and cooperative near field coupling between neighbouring dipoles, which gives rise to cooperative action thus determining the macroscopic properties. Examples involve transparent conducting metal coatings, perfect plasmonic absorbers, active plasmonic and photoswitchable composites.

Acknowledgements: Financial support by the Initiative Networking Fund of the Helmholtz Association and DFG within the Collaborative Research Centers SFB 677 are acknowledged.

On-Substrate Fabrication of Porous Al-Oxide Templates with Tunable Pore Diameters and Interpore Distances

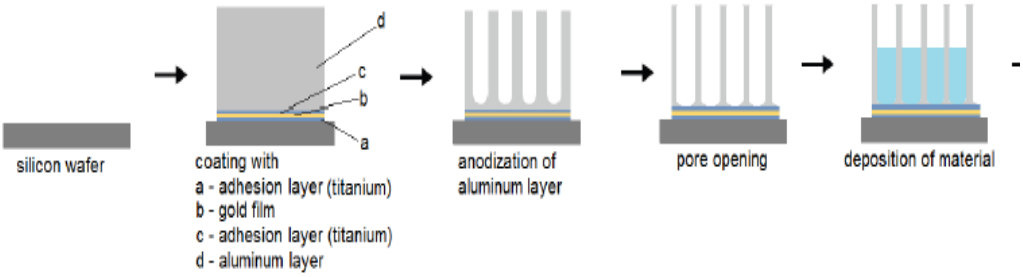
Nele Berger[1], Horst-Günter Rubahn[2],
Salah Habouti[1] and Mohammed Es-Souni[1]

[1]Institute for Materials & Surface Technology, University of Applied Sciences, Kiel, Germany
[2]NanoSYD, Mads Clausen Institute, University of Southern Denmark, Alsion 2, 6400 Sønderborg, Denmark

Porous aluminum oxide (PAO) thin films can be used as templates for the fabrication of nanorod arrays of different materials. These arrays can be used for different purposes such as SERS or electrochemical energy storage devices. Different applications can require different morphologies of nanorod arrays. For instance, if a maximization of the surface area is desired, the array must consist of nanorods as small and closely spaced as possible.

This work is focused on the on-substrate fabrication of PAO templates by anodization of a thin aluminum film deposited directly on the substrate. These on-substrate templates can be used for creating free-standing nanorod arrays by deposition of different materials followed by the removal of the template as shown in the cartoon below.

The morphology of these templates is influenced by the variation of different parameters during the fabrication process. The interpore distance can be tuned by choice of electrolyte used for anodization, its concentration, and the applied voltage. The diameter of the pores (and thus the nanorods) and wall thickness between them relates to the acid, temperature, and time used for pore widening.


d
c
b
a
silicon wafer
coating with
a - adhesion layer (titanium)
b - gold film
c - adhesion layer (titanium)
d - aluminum layer
anodization of
aluminum layer
pore opening
deposition of material

Properties and Applications

Time: 16.40 – 18.00

Room: Lecture hall 2

Chair: Mato Knez

Friday, 2015-09-11	16.40	Talk	Properties and applications	Lecture hall 2

Supported Porous Carbon and Carbon-CNT-Nanocomposites for Supercapacitor Applications

Dimitri Schopf and Mohammed Es-Souni

Institute for Materials & Surface Technology, University of Applied Sciences, Kiel, Germany

Template-free porous PVDF films are processed on thermally resistant substrates using a precursor solution (see reference 1). The solution can be easily modified with multi-walled carbon nanotubes (MWCNT) to yield porous PVDF-MWCNT-nanocomposite films. Subsequent pyrolysis of the films at the fairly low temperature of 550°C leads to amorphous porous nanocarbon films (see reference 2) or nanocarbon-MWCNT-nanocomposites. The complete procedure is shown in Fig. 1. All films are characterized by SEM, RAMAN and XRD. The application of these films as supercapacitors is explored with supercapacitance values ranging from 80 to 360 F/g (in 1M KOH), depending on microstructure. In all cases long term charge-discharge stability is demonstrated.

Friday, 2015-09-11	16.40	Talk	Properties and applications	Lecture hall 2

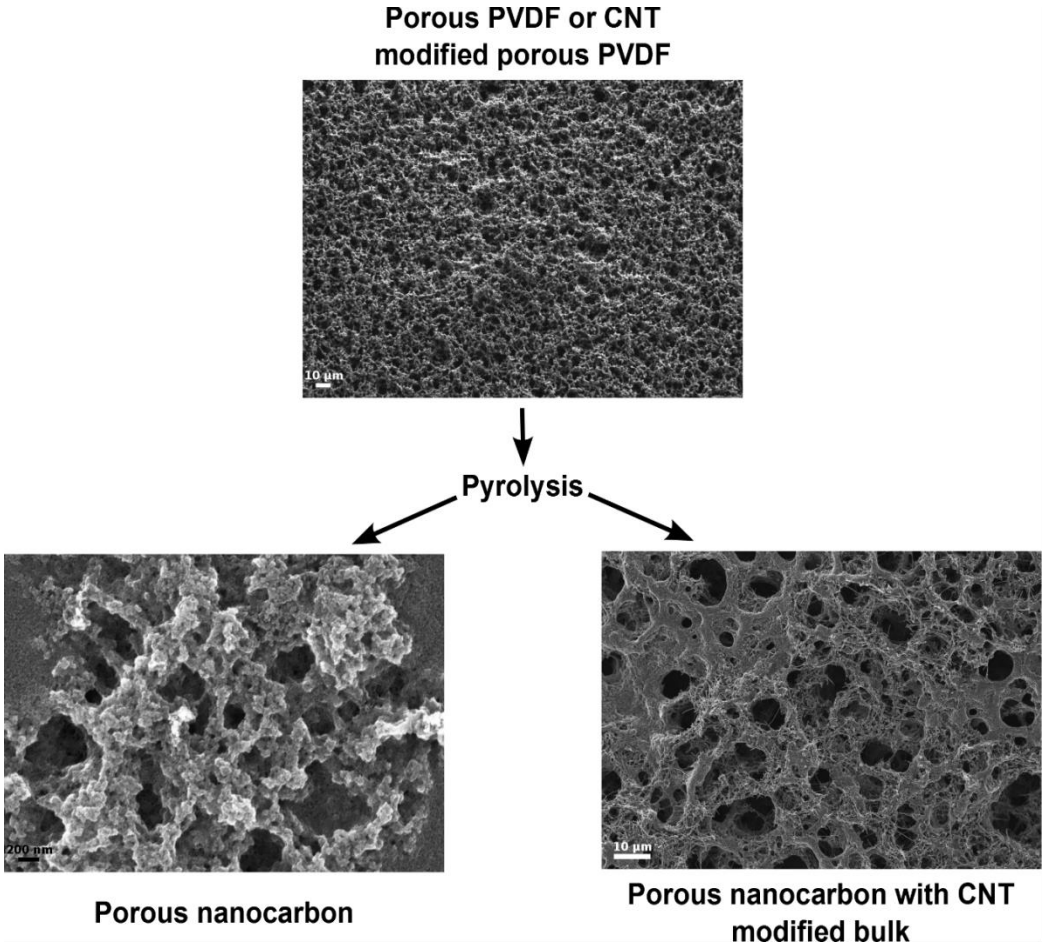


Fig. 1 Proceeding for supported porous carbon films

[1] M. Es-Souni, M. Es-Souni, and M. Dietze, *RSC Adv.*, 2011, **1**, 579-583
[2] M. Es-Souni, D. Schopf, C.-H. Solterbeck and M. Dietze, *RSC Adv.*, 2014, **4**, 17748

Friday, 2015-09-11	17.00	Talk	Properties and applications	Lecture hall 2

Preparation of Antibacterial and Conductive Textiles Impregnated with Graphene Oxide, Graphene and Metallic Nanoparticles

Ouadil Boubker[1,2], Zahouily Mohamed[1], Cherkaoui Omar[2], Rajaa Ait Mhand[1] and Mohamed Safi[1]

[1]Laboratoire de Matériaux, Catalyse et Valorisation des Ressources Naturelles, URAC 24, Faculté des Sciences et Techniques, Université Hassan II, Mohammedia B. P. 146, 20650, Morocco
[2]Higher School of Textile and Clothing Industries, Laboratory REMTEX, Km 8, Route d'El Jadida; BP 7731, Oulfa, Casablanca, Morocco

A simple approach has been reported to fabricate an electro-conductive textile by impregnating graphene oxide (GO) and metallic nanoparticles onto fabrics, the as prepared fabric was then reduced through chemical method using different reducing agents in order to convert graphene oxide into graphene. The fabrics were characterized using Fourier transform infrared (FTIR) spectra. UV–Vis spectroscopy. Color coordinates were determined by color measurement software using the CIE L* a* b*.Tensile strength and elongation of the samples were evaluated using a MESDAN LAB instrument. The thermal properties of the samples were characterized by Thermogravimetric analysis (TGA). After reduction, the modified textiles show an important conductivity and mechanical performance. The antibacterial activity was evaluated against both Gram-negative (Escherichia coli) and Gram-positive (Staphylococcus aureus) bacteria and the results indicated that fabrics expressed have activity against strains (E. coli and Staphylococcus) of different morphology and different GRAM. The present work contributed a facile strategy for graphene modified polyester fabric with multifunctional properties.

Friday, 2015-09-11	17.20	Talk	Properties and applications	Lecture hall 2

Effect of Microstructure on the Electrical Properties of TiO_2 Thin Films Deposited by Chemical Spray Pyrolysis

Albert Juma[1,2], Ilona Oja Acik[1], Arvo Mere[1] and Malle Krunks[1]

[1]Laboratory of Thin Film Chemical Technologies, Department of Materials Science, Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia
[2]Department of Physics and Astronomy, Botswana International University of Science and Technology, Private bag 16, Palapye, Botswana

The electrical properties of TiO_2 thin films deposited by chemical spray pyrolysis from the solution containing various molar ratios of titanium (IV) isopropoxide: acetylacetone onto Si substrates with a thermally grown oxide layer were investigated using current-voltage characteristics and impedance spectroscopy. The electronic transport properties were analyzed in relation to the changes in microstructure induced during annealing up to a temperature of 950°C. The dominant conduction mechanism in the SiO_2/TiO_2 dielectric stack was the Poole-Frenkel with trap barrier heights of 0.40 – 0.56 eV depending on the annealing temperature. The dielectric relaxation in the system at the interface with the metal electrodes dominated in the as – deposited samples and could be described by a constant phase element in the equivalent circuit. After annealing at 800°C or higher temperatures, the electrical properties were mainly affected by the dielectric relaxation due to the grains and grain boundary contributions. The strong correlation between microstructural changes and electronic properties will also be discussed.

Friday, 2015-09-11	17.40	Talk	Properties and applications	Lecture hall 2

Effect of Different Molarities on Structural and Optical Properties of ZnO Thin Films Elaborated by Spin Coating Method

G. El Hallani[1], N. Fazouan[1], A. Liba[1], M. Sajieddine[1] and L.Laanab[2]

[1]Physical Materials Laboratory, University of Sultan Moulay Slimane, Beni Mellal, Morroco
[2]Solids Physic Laboratory, University of Mohamed V, Rabat, Morroco

In this work the effects of varying molarities on structural, morphology and optical properties of ZnO thin films were investigated. The films were growth on glass substrates using spin coating method and were thermally annealed at 500˚C. Thin films produced at 0.25 to 1 M have been analyzed using X-ray diffraction (XRD) and scanning electron microscopy (SEM) to investigate their crystallinity and surface morphology. The optical absorbance and transmittance measurements were recorded by using a double beam spectrophotometer. The results show that the ZnO thin films are polycrystalline and exhibit the hexagonal würtzite structure with a preferential orientation along [002] direction for all samples. The crystallite sizes and thickness of thin films are increased with increasing sol concentration. The films present an average optical transmittance between 90% to 95% in the visible range with some interference fringes. The energy gap was evaluated and shows a decrease when the precursor concentration increases. These results reveal that the precursor concentration in the sol–gel spin coating process exerts a strong influence on the properties of the ZnO films.

Numerical Studies

Time: 16.40 – 18.00

Room: Seminar room 1

Chair: Jost Adam

Friday, 2015-09-11	16.40	Talk	Numerical studies	Seminar room 1

Optical Performance of ZnO and ZAO (ZnO:Al) Thin Films Prepared by Reactive Magnetron Sputtering: Experimental and ab initio Study

Houda Ennaceri[1,2], Mourad Boujnah[1], Asmae Khaldoun[2], Tristan Köhler[3], Ahmed Ennaoui[4] and Abdelilah Benyoussef[1]

[1]Department of Physics, University Mohammed V, Rabat, Morocco
[2]School of Science and Engineering, Al Akhawayn University, Ifrane, Morocco
[3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany
[4]Qatar Environment and Energy Research Institute (QEERI), Qatar

In this study, intrinsic zinc oxide (i-ZnO) and aluminum-doped zinc oxide (AZO) thin films were grown by mean of radio frequency magnetron sputtering on glass and FTO substrates at a chamber temperature of 275°C. The AZO layers were deposited from a ZnO target mixed with 2 wt% Al_2O_3. A wide range of characterization techniques such as X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), surface photo-voltage measurements (SPV) and Ultraviolet-Visible-Near Infrared spectrum were used to characterize the ZnO and ZAO layers. The experimental results show that the transmittance of the AZO films is above 80% in the visible and near infrared range, which is higher than the transmittance of pure ZnO films of the same thickness. The ab intio calculations were conducted based on the full-potential linearized augmented plane wave (FP-LAPW) method, which has been performed to solve the Kohn-Sham equations within the Density Functional Theory (DFT), and was implemented in WIEN2k package. The ab initio calculations were conducted using the Gradient Generalization Approximation (GGA) and the modified Becke Johnson (mBJ) potential, respectively. The optical band gap, as well as the experimental optical parameters of the deposited layers of ZnO and ZAO were studied (absorption coefficient, refractive index, extinction coefficient and dielectric constants), which were in good agreement with the calculated parameters using ab-initio calculations.

Friday, 2015-09-11	17.00	Talk	Numerical studies	Seminar room 1

First Principles Study on the Electronic and Optical Properties of Si and Al Co-Doped Zinc Oxide for Solar Cell Devices

A. Abbassia[1], A. El Amranib[2], H. Ez-Zahraouya[1], A. Benyoussefa[1] and Y. El Amraouia[1]

[1]Laboratory of Magnetism and High Energy Physics (URAC 12) B.P. 1014, Faculty of Sciences, University of Mohammed V, Rabat, Morocco.
[2]LPSMS, Dept. of Phys. FST, University My Ismail BP 509, Boutalamine, Errachidia, Morocco

Electronic and optical properties of zinc oxide ZnO co-doped with silicon (Si) and aluminum (Al), as $Zn_{1-2x}Si_xAl_xO$ ($0 \leq x \leq 0.0625$) original structure form, are investigated by the first principles calculations based on the density functional theory (DFT). The optical constants as well as dielectric functions are investigated with the full potential-linearized augmented plane wave (FP-LAPW) method and the generalized gradient approximation (GGA) by Wien2k package. The complex dielectric functions, refractive index and band gap of the pure as well as doped and co-doped ZnO were investigated, which are in good agreement with the available experimental results for the undoped ZnO. In addition, the maximum optical transmittance of the co-doped ZnO of about 95 % was achieved; it is higher than that of pure ZnO. Thus, we showed for the Si-Al co-doped ZnO with x=0.0315 that the optical transmittance covers a larger range in the visible light region. In addition, an occurrence of important energy levels around Fermi levels was showed, which is mainly due to aluminum atoms that leading to an overlap between valence and conduction bands, and consequently to the significant conductor behavior of the Si-Al co-doped ZnO. The $Zn_{1-2x}Si_xAl_xO$ structure reveals promising optical and electronic properties, and it can be investigated such as good candidates for practical uses as transparent and conducting electrodes in solar cell devices.

Friday, 2015-09-11	17.20	Talk	Numerical studies	Seminar room 1

Ab initio Comparative Study of Scintillating Crystals LaX_3 with X = (F, Br and I) using mBJ Exchange-Correlation Potential

M. Boujnah[1], M. Y. Messous[2], H. Labrim[2], A. Benyoussef[1,3], A. Ferreira da Silva[4] and A. El Kenz[1]

[1]Laboratory of Magnetism and Physics of High Energy, Department of Physics, B.P. 1014, Faculty of Sciences, Rabat, Morocco
[2]National Center for Energy, Sciences and Nuclear Techniques, B.P 1382 R.P 10001 Rabat, Morocco
[3]Institute of Nanomaterials and Nanotechnolog, MASCIR Foundation, Av. of the royal army, Madinat el irfane, 10100 Rabat, Morocco
[4]Instituto de Física, Universidade Federal da Bahia, Campus Universitário de Ondina, 40210 340 Salvador, Bahia, Brazil

The basic structural, electronic and optical properties of the binary lanthanum trihalides (F, Br and I) were studied using the density functional theory within the Generalized Gradient Approximation (GGA) for exchange and correlation functional. The modified Becke-Johnson (mBJ) method was also applied with the primary goal of improving the electronic structure description of this group of materials. Energetically, the result shows that $P6_3$ cm and P3c1 - LaF_3 are stable than $P6_3$/mmc and more stable than the $P6_322$ case. After calculation taking in account the most stable phase of the considered compound, we find that the mBJ functional gives greatly improved band gaps and optical properties in this class of materials. Furthermore, we find that LaI3 has the smallest band gap of the compounds family. The calculation in the 0-10 eV range energy reveals that all optical properties of Fluoride Lanthanum have small variation and offer higher refractive index and they are less reflective.

Friday, 2015-09-11	17.40	Talk	Numerical studies	Seminar room 1

Numerical Study of the Adsorption and the Diffusion on the Clean (1×1) Unreconstructed and (1×2), (1×3) and (1×4) Reconstructed Pt (110) Surfaces

I.Matrane[1], E. El koraychy[1], K. Sbiaai[2,3], M. Mazroui[1] and Y. Boughaleb[1,3]

[1]*Laboratoire de la Physique de la Matière Condensée (URAC10), Faculté des Sciences Ben M'sik, B.P. 7955, Université Hassan II Casablanca, Morocco*
[2]*Université Hassan I, Faculté Polydisciplinaire de Khouribga, 26000 Settat, Morocco*
[3]*Laboratoire de l'ingénierie des Matériaux et Biosciences, Ecole Normale supérieure, Université Hassan II, Ain Chock, Casablanca, Morocco*

Adatom diffusion on metal surfaces has been intensively studied over the previous several decades both theoretically and experimentally because of the potential applications in several area such as in electronic devices (nanotechnology), chemical reactions, catalysis and micro-semiconductors. Despite of increasing the research in this area, it still many unresolved issues because the complexity of the phenomena and each system has an own behavior.

The present work was focused on the investigation of the diffusion and the adsorption of Pt and Au adatoms on the ideal (1×1) and (1×2), (1×3) and (1×4) missing row structures of Pt (110) surfaces. For each geometry, two systems are considered: homogenous Pt/Pt and heterogeneous Au/Pt systems. The multilayer and adatom relaxation trends were examined. To check the validity of our findings, we have compared our results with simulated data of the density-functional theory and an excellent agreement was found for this specific study of the relaxation. On the other hand, the static energy barrier for hopping diffusion and the adsorption energy were calculated for the perfect and missing row reconstructed geometries. The analysis provides an interesting insight and a precious idea about the geometry influence on the adsorption and the diffusion on the missing-row reconstructed surfaces.

Poster session 2

Friday, September 11th, 2015

Time: Afternoon 18.00 – 19.00

Influence of Sol Concentration and Annealing Temperature on the Structural and Optical Properties of Nanocrystalline ZnO Thin Films Synthesized by the Sol-Gel Method

Rabab Bekkari[1], Boujemaâ Jaber[2] and Larbi Laânab[1]

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The controlled synthesis of ZnO nanoparticles and in-depth understanding of the physical properties are the key issue for the future development of ZnO-based devices. ZnO films can crystallise in various orientations which strongly depend on the deposition technique, sol concentration and other factors [1]. The quality of the ZnO film is typically determined by its crystalline orientation, surface uniformity, transparency and conductivity. Among all of these parameters, the crystalline orientation is the most important parameter to optimize when seeking to develop ZnO films with piezoelectric properties [1, 2]. It is around this perspective that turns our project in which we project to develop transducers based on ZnO material. To excite several modes we need films presenting different orientations. In this context, the main objective of this work is to study the influence of sol concentration and annealing temperature on the structural and optical properties of Nanocrystalline ZnO thin films.

ZnO thin films are deposited successfully on silicon substrate by sol-gel spin coating method by varying precursor concentrations and annealing temperature. The structural properties of ZnO thin films were investigated by X-Ray Diffraction (XRD) and Scanning Electron Microscope (SEM) techniques. The XRD spectra showed that the films were of hexagonal wurtzitein structure. The grain size of crystallites increases with increase in Zn concentrations and in annealing temperature ranging from 10 to 40 nm. SEM analysis confirmed that all the ZnO films have granular, uniform and nano-seized grains. The UV

visible spectral study showed a direct band gap value in the range of 3.27 eV to 3.32 eV for the studied Zn concentration and annealing temperature prepared Zinc Oxide thin films.

[1] M.F. Malek , M.H. Mamat , Z. Khusaimi , M.Z. Sahdan , M.Z. Musa , A.R. Zainun , A.B. Suriani, N.D. MdSin, S.B. Abd Hamid, M. Rusop, Sonicated sol–gel preparation of nanoparticulateZnO thin films With various deposition speeds: The highly preferred c-axis, Journal of Alloys and Compounds 582 (2014) 12–21
[2] D. Bao, H. Gu, A. Kuang, Sol–gel-derived *c*-axis oriented ZnO thin films, Thin Solid Films 312 (1998) 37

Physical Properties of Gd Doped ZnO Thin Films Grown by Spray Pyrolysis

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Undoped ZnO, Gd doped ZnO (GZO) thin films were prepared by chemical spray pyrolysis method at 350° C on glass substrates. the effects of gadolinium doping on structural, morphological, optical and electrical properties as function of dopant concentration has been studied. X-ray analysis showed that the films are polycrystalline fitting well with hexagonal wurtzite structure and have preferred orientation in [002] direction. The AFM analysis showed that the grain size as well as the roughness of the Gd doped ZnO films constantly decreases with increasing dopant content. The deposited films showed an average optical transmittance around 85% in the visible region. The optical band gap of the ZnO:Gd films decreases from 3.27 eV to 3.18 eV as dopant content increases. Hall Effect measurements revealed that the Gd doping induces an increase in the electron concentrations, making the films heavily n type. The electrical conductivity, mobility carriers and carrier concentration of the films are increased with 1.5 % Gd doping concentration.

Structural, Electronic and Thermal Properties of Wurtzite ZnO Structure

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First-principles calculations for structural, electronic and thermal properties of ZnO compounds in the wurtzite structure, using a full relativistic version of the full-potential augmented plane-wave (FP-LAPW) method based on density functional theory, within the local density approximation (LDA) and the generalized gradient approximation (GGA), have been reported. Furthermore, band structure calculations have been investigated by the alternative form of GGA proposed by Engel and Vosko (GGA-EV) and modified by Becke-Johnson exchange correlation potential (MBJ). All calculated equilibrium lattices (a, c and μ), bulk modulus and band gap are find in good agreement with the available reported data. The quasi-harmonic Debye model, using a set of total energy versus volume calculations obtained with the FP-LAPW method which is applied to study the thermal properties. Temperature effects on the structural parameters, thermal expansions, heat capacities and Debye temperatures are determined from the non-equilibrium Gibbs functions.

[1] S. Labidi, A. Lakel, M. Labidi and R. Bensalem, CHIN. PHYS. LETT 31, (2014) 046104.
[2] M. Labidi, S. Labidi, F. El Haj Hassan, M. Boudjendlia, R. Bensalem, Mater. Sci. Semicond Process 16 (2013) 1853-1858

First Principles Study of (Mg, Al)-Codoped ZnO with GGA and mBJ Approximations

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The physical properties such as structural, electronic, optical and electrical characteristics of the co-doped ZnO system $Zn_{1-x-y}Mg_xAl_yO$ were studied. To determine the structural parameters as well as the structure stability, we use Gaussian and plane waves basis set method implemented in CP2K code. Combined to this code, the modified Becke–Johnson potential (mBJ) approximations implemented in Wien2k code was introduced to calculate the other properties. We have found that the magnesium (Mg) doped ZnO enhancing the optical properties and induce a blue shift in optical band gap of zinc oxide but has reduced its electrical properties. The incorporation of aluminium (Al) in Mg doped ZnO achieve good electrical conductivity and high transmittance of transparent conductive ZnO. These results make $Zn_{1-x-y}Mg_xAl_yO$ system as a suitable candidate in electronic transparent devices.

First Principles Calculations of the Structural, Elastic and Thermal Properties of ZnO in Zinc Blende Structure

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First-principles calculations are performed to investigate the structural, elastic and thermal properties of ZnO in Zinc blende structure using the full-potential linearized augmented plane wave method. In this approach, the generalized gradient approximation (GGA) of Perdew et al. was used for exchange correlation potentials. Results are given for lattice constant, bulk modulus and elastic constants are in agreement with experimental and theoretical data. Through the thermal effect on some macroscopic properties was investigated using the quasiharmonic Debye model.

First Principal Study of Hydrogen Storage Proprieties of Double Substituted Mg Based Hydrides $Mg_{14}TMLiH_{32}$, (TM=Sc, Ti, V, Cr, Y, Zr, Nb, Mo)

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[3]Centre National de l'Energie, des Sciences et des Techniques Nucléaires, Rabat, Morocco
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[5]Hassan II Academy of Science and Technology, Rabat, Morocco

Ab-initio calculations are carried out to investigate the improvement of hydrogen storage properties, in Mg-based hydrides, through a double substitution ($Mg_{14}TMLiH_{32}$, TM = Sc, Ti, V, Cr, Y, Zr, Nb, Mo). The calculations are performed using the all-electron full-potential local-orbital minimum-basis scheme (FPLO9.00-34). Our results indicate a decrease of the heat of formation and desorption temperature, while preserving the gravimetric storage capacity around 7.6wt%, which is due to the second substitution with Li (Li is characterized by its light weight and small radius). Discussions of electronegativity, the charge exchange and the density of states are done, to offer more possible explanations to our results.

Ab initio Study of Effects of B (Bsub,Bins) Substituted and Insertion Tm (Sr,Ca) Co-Doping on Destabilizing of MgH_2

Mustapaha Abdellaoui

Faculty of Science, Mohammed V University Rabat, Marocco

In this paper we study the B-sub$TmMg_4H_{12}$ and B-ins$TmMg_4H_{12}$ systems employing the density functional theory (DFT) within the plane wave and pseudo potential method. We discuss the chemical bond nature from the total and partial density of states (DOS) along with Charge density analysis. It is shown an increasing of covalent character of hydrogen: Mg_6H_{12}→B-sub$TmMg_4H_{12}$. In addition, we calculate the heat formation of both hydride compounds for an application in hydrogen storage domain.

First Principal Calculations of Optical and Electrical Properties in F and Al Doped TiO_2 DMS.

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Using the First-principles calculations and WIEN2K codes based on Linear Augmented Plan Wave (LAPW) method, we investigate the structural, electronic, electrical and optical properties of pure and F or Al atoms doped TiO_2. The aim is to find an optimal material to be used in photovoltaic solar cells. We optimized crystal structures (by the relaxation method), band structures, electrical and optical gap partial and total densities of states (DOS), absorption spectra, optical conductivity, reflectivity, to allow the material to make the most of the visible light and the refractive index on the wavelength. Comparison of the calculated and experimental results is discussed. Electrical conductivity is also investigated using the Boltzman transport properties implemented in the Boltztrap code. And the results indicate an electrical conductivity well optimized.

First Principles Calculations of GaN and AlN Nanosheets

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First principles calculations were performed to study the electronic structures of gallium nitride (GaN) and aluminum nitride (AlN) nanosheets in order to understand the influence of sheet stacking (in terms of thickness) on structural and electronic properties, as well as the relative stabilities of fully and partially hydrogenated nitride nanosheets. Unlike bare GaN and AlN nanosheets terminating with polar {0001} surfaces, their hydrogenated counterparts preserve the initial wurtzite configuration. Specifically, the dielectric function, absorption coefficient, optical conductivity, extinction index, reflectivity and their fraction index of both type of nanosheets are calculated for both parallel and perpendicular electric field polarizations. The results show that the optical spectra are isotropic along these two polarizations. Optical conductivity in both the parallel and the perpendicular electric field starts with an indirect gap (instead of indirect gap for bulk counterparts) which confirms that nitride nanosheets have a semiconductor property.

Numerical Simulation of the Filling Phase of the Microinjection Process with the Level Set Method

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The present work concern the analysis of numerical simulation of non- Newtonian fluid flows during filling phase in micro molding process. In this process, the polymer melt is injected from the gate of the cavity in which initially filled by the air, resulting in a two phase flow of polymer-air interface. The level set method is used in order to track the interface, which will be coupled with Navier Stokes and energy equations. A finite element method is used to solve these equations, which gave a remarkable and fine precision for the reconstruction of the interface. The results show clearly the expected fountain flow effect. Temperature, velocity, pressure and viscosity fields are calculated versus time and discussed.

Numerical Study by the Meshless Method LRPIM of Shape Parameter in Radial Basis Function in Linear Elasticity

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The method LRPIM is a Meshless method with properties of simple implementation of the essential boundary conditions and with the lower cost than MLS methods. This method was proposed to overcome the singularity associated to polynomial basis by using radial basis functions. In this paper, we present a study of a 2D problem of an elastic homogenous rectangular plate problem by using the method LRPIM. Our numerical investigations concern the influence of different shape parameters on the domain convergence and accuracy and by using the radial basis function the thin plate spline. It also presents a comparison with numerical results for different materials and the convergence domain by precising maximum and minimum values as a function of distribution nodes number. Numerical results agree with the analytical solution of the deflection.

Antisite Disorder Study by Monte Carlo Simulation of the Double Perovskite Sr_2CrReO_6

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The Double Perovskite (DP) Sr_2CrReO_6 is an interesting material in spintronics thanks to its high Curie temperature (Tc=635 K). The antisite disorder is a defect that affects the spin polarization and the Curie temperature of all PDs. We conducted this work by Monte Carlo simulation to study the effect of antisite disorder on this compound for two cases: Cr-excess expressed by $Sr_2Cr_{1+x}Re_{1-x}O_6$ and Re-excess expressed by $Sr_2Cr_{1-x}Re_{1+x}O_6$. This simulation has transformed the concept of antisite conceived as defect, into a tool for explaining the role of transition metals, namely Cr and Re, in the stability and the magnetic performance of the compound Sr_2CrReO_6. This simulation allows positioning the Cr as a key element in determining the high Curie temperature and the ferromagnetic stability. The effect of crystalline field of Re regarding disorder rates in the disordered sublattice was also explored.

Spontaneous Polarization, Magnetic and Electronic Properties of $BiXO_3$(X=Co, Mn, Fe, V, Zn): First Principles Study

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Spontaneous polarization, electronic, magnetic and Optical properties of $BiXO_3$ with X = Co, Fe, Mn, V and Zn have been studied using the Full Potential Linear Augmented Plane Wave (FPLAPW) method with the generalized gradient approximation (GGA)and modified beak Johnson approximation (mBJ),, implemented in the WIEN2K code .The investigation show that $BiXO_3$ with X= Co, Fe ,Mn, Zn is stable in the antiferromagnetic state while for $BiVO_3$ the magnetic stability was shown in the ferromagnetic state. With the mBJ approximation, the transfer of charge between p states of oxygen and d states of Co and Fe show that the band gap is equal to 1.7 eV for $BiCoO_3$ and 2.6 eV for $BiFeO_3$, which is in good agreement with experimental results. The existence of these elements Co, Fe, Mn, V make $BiXO_3$ non-absorbent compound. However, for Zn this structure make it as absorbent compound especially in the visible light. We note that the spontaneous polarization is calculated with Berry phase BI and was found very close and comparable with other works. This results result that can be exploited in different optoelectronic and magneto-optic applications.

Magnetic Properties of Heavy Fermions Compound URu_2Si_2: Ab initio Calculations and Monte Carlo Simulation

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On the basis of ab initio calculations, Mean Field Approximation and Monte Carlo Simulation, the phase diagram and the magnetic properties of the heavy fermions compound URu_2Si_2 have been studied. Using the Ising model, the transition temperature and the critical exponents are obtained in the framework of Monte Carlo simulation, the exchange couplings of the Ising model are deduced from ab initio calculations. The obtained results lead to a quantitative agreement with the experimental temperature transition.

Magnetism of Size Effect in Graphene Nano-Islands: A Monte Carlo Study

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The double-wall cubic metal nanotube consists of the ferromagnetic spin-5/2 inner shell and spin-5/2 surface shell. It is of the ferrimagnetic exchange coupling between two shells. The magnetization, susceptibility, the internal energy and the specific heat have been investigated by using the Monte Carlo simulations. Some interesting phenomena have been found in the thermal variations of the system. Magnetization appears two or three compensation points in certain parameters. It is an unconventional ferrimagnetic behavior in the nanotube. The shapes of total magnetization and the magnetic susceptibility are great influenced by the surface exchange coupling. The magnetic hysteresis cycles are obtained for different temperature, crystal field and exchange interaction. Some results of nanotube may have potential applications in different research fields, such as electronics, optics, mechanics, and even biomedicine and molecular devices.

Dynamic Compensation Temperatures and Hysteresis Behaviors of a Mixed Spin Ising Double Walled Ferromagnetic Nanotubes

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Using the Monte Carlo simulation, the dynamic compensation and critical temperatures of a ferromagnetic or ferrimagnetic double walled nanotubes are studied within the Ising model with mixed spins S_A=1 and S_B=3/2 in the presence of the crystal and oscillating external magnetic fields. The effects of the exchange interactions, the time-dependent oscillating external magnetic field, the crystal field on the thermal behavior of the dynamic sub lattice magnetizations and the total magnetization, specific heat and the internal energy of a double walled nanotubes are studied. Our theoretical predictions may be a reference for future experiment studies of the nanostructures.

Phase Diagrams of Spin-1 Ashkin-Teller Model with Crystal Field and Transverse Field

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We study the spin-1 Ashkin Teller model on hypercubic lattice by using the mean field theory (MFT), tree new phase diagrams are found by varying the crystal field, on the other hand we have found tree new phase diagrams within different Transverse Field. Multicritical behavior is studied as a function of four-spin interaction coefficient. Moreover, in order to assured the existence of the phase diagrams we plotted the variation of Transverse Field as a function of crystal field in which we have specify the results.

Changing the Magnetic and Optical Properties of (Ga, Fe)N and (Ga, Co)N by Alloying with Oxygen

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GaN diluted magnetic semiconductor (DMS) compounds have been extensively investigated as good candidates for optoelectronic devices, such as detectors and emitters, as well as high-power electronics and high-efficiency solar cells. Additionally, high Curie temperatures and room-temperature ferromagnetism have been predicted in GaN-doped with transition-metal elements, such as Fe, Co, Mn and Cr which in principle opens the door for room temperature, semiconductor-based spintronic applications.

In this paper, the first-principles spin-density functional calculations have been used to show that the magnetic properties of $(Ga_{0.94}Fe_{0.06})N$ and $(Ga_{0.94}Co_{0.06})N$ can be changed from disorder local moment state to ferromagnetic state by replacing ~2% of the nitrogen atoms with oxygen atoms. The estimated curie temperatures are much higher than the room temperature which indicates the room temperature ferromagnetism can be realized by oxygen doping. Moreover, the optical absorption spectra obtained by ab-initio calculations confirm the ferromagnetic stability based on the charge state of magnetic impurities. $(Ga_{0.94}Fe_{0.06})N_{0.98}O_{0.02}$ and $(Ga_{0.94}Co_{0.06})N_{0.98}O_{0.02}$ ferromagnetic DMS exhibit half-metallic behavior, which is suitable for spintronics applications.

Magnetic and Magneto-Optical Properties of Doped and Co-Doped CdTe

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On the basis of ab-initio calculations, the magnetic properties of CdTe doped with transitions metals Mn, Fe and co-doped with both, which make this material a possible candidate for spintronic applications, have been investigated. Moreover, the density of state DOS for different dopants concentrations have been calculated and plotted with the energy diagram, we studied the experimental results of the doping of CdTe and determined which one is responsible of the magnetism appearing ,Mn or Fe ,then we observed the effect of the codoping with Mn and Fe. We found that the iron Fe does not contribute strongly in the magnetism but affect the optical properties of the DMS, so in experimental work we find that a low concentration of Fe improves well the magneto-optical properties such as the faraday rotation. We also investigate the microscopic behavior of electrons by studying its electronic structure and density of states.

Magnetic Properties and Phase Transition in Transitions Metal Doped Semiconductor GaN

Y. Sbai, A. Ait Raiss , E. Salmani , L. Bahmad and A. Benyoussef

On the basis of ab-initio calculations and Monte Carlo simulations the magnetic and electronic properties of Gallium nitride (GaN) doped with the transition metal Manganese (Mn) were studied. The ab initio calculations were done using the AKAI-KKR-CPA method within the Local Density Approximation (LDA) approximation. We doped our Diluted Magnetic Semiconductor (DMS), with different concentrations of magnetic impurities Mn and plotted the density of state (DOS) for each one. Showing a half-metallic behavior and ferromagnetic state especially for $Ga_{0.95}Mn_{0.05}N$ making this DMS a strong candidate for spintronic applications. Moreover, the magnetization and susceptibility of our system as a function of the temperature has been calculated and give for various system size L to study the size effect. In addition, the transition temperature was deduced from the peak of the susceptibility. The Ab initio results are in good agreement with literature especially for (x=0.05) of Mn which gives the most interesting results.

Structural and Magnetic Study of $Co_{(1-x)}Ni_xFe_2O_4$ Nanoparticles Synthesized by the Sol-Gel Method

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The multiferroic materials are compounds that exhibit exceptional properties. Indeed, in these systems there is a magneto-electric coupling, that is to say a coupling between their electrical and magnetic properties. It is also possible to control the electric polarization by application of a magnetic field, and vice versa it is possible to control the magnetic state by applying an electric field.

In this paper, we are going to present the structural and magnetic properties of $Co_{1-x}Ni_xFe_2O_4$ nanoparticles with x from 0.1 to 0.9 in steps of 0.1. The nanoparticles are prepared by the sol-gel method, structural analysis by X-ray diffraction has lead to determination of the spinel structure of the prepared samples. Transmission electron microscopy analysis was carried out to reveal the local microstructure of the particles, the image reveals that particles are in nanometer range (6 - 8 nm), with spherical shape. The investigation of the magnetic measurements has been done using a Magnetic Properties Measurement System (MPMS).

Synthesis and Magnetic Properties of Cobalt Ferrite Nanoparticles Doped with Neodymium and Tin

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In this work we report the synthesis, the microstructural characterization and the magnetic properties of $Co_{0.5}M_{0.5}Fe_2O_4$ (M= Nd and Sn) spinel ferrites nanoparticles prepared by co-precipitation method. The average size of composite nanoparticles for $Co_{0.5}Nd_{0.5}Fe_2O_4$ and $Co_{0.5}Sn_{0.5}Fe_2O_4$ are 10 and 13 nm, respectively. All samples prepared possess ferrimagnetic phase. The blocking temperatures of cobalt spinel ferrites doped with neodymium and tin are found to be approximately 350 K and 370 K, respectively. The observed magnetic moment and coercive field's values of Cobalt spinel ferrites doped with neodymium sample are higher than $Co_{0.5}Sn_{0.5}Fe_2O_4$.

Thermodynamic Properties and Hysteresis Behaviors of a Mixed Ferrimagnetic Nanowire

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In this work the mixed spins Ising nanowire model consisting of a spin-1 ferromagnetic core which is surrounded by a spin-1/2 ferromagnetic surface shell is studied in the presence of the magnetic and crystal fields using of the Monte Carlo Simulation (MCS) based on the heat bath algorithm. We have examined the effects of the surface and crystal field on the critical and compensation temperatures. The thermodynamic properties, the hysteresis behaviors are also studied and for the appropriate values of the system parameters, the compensation point and multi-loops are found.

Morning sessions

Saturday, September 12th, 2015

Ferroic Materials and Structure

Time: 09.00 – 11.40

Room: Lecture hall 2

Chair: Abdelilah Benyoussef

Saturday, 2015-09-12	09.00	Talk	Ferroic materials and structure	Lecture hall 2

Ferroelectric and Ultrasonic Studies on Polymer Based P(VDF-TrFE) Composites with PZT, BTO and CFO Inclusions

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Piezoelectric materials can be doped with various fillers in order to modify their properties. In this work we present experimental study on the impact of piezoelectric fillers on the ferroelectric and the ultrasonic properties of a ferroelectric conventional ferroelectric copolymer based composite. We used polyvinylidene fluoride / trifluoroethylene (P(VDF-TrFE)) copolymer with a molar ratio 70/30 as the composite matrix to be filled with PZT family $(Pb_{0,75}Ba_{0,24}Sr_{0,01})(Zr_{0,53}Ti_{0,47})O_3$ (BPZT), $BaTiO_3$ (BTO) and $CoFe_2O_4$ (CFO) fillers. $(Pb_{0,75}Ba_{0,24}Sr_{0,01})(Zr_{0,53}Ti_{0,47})O_3$ (BPZT), $BaTiO_3$(BTO) and $CoFe_2O_4$ (CFO) fillers. Composites of different piezoelectric filler concentrations are studied (up to 50 vol. % in case of BPZT, 15 vol. % in case of BTO, 11 vol. % in case of CFO). The impact of filler concentration on the shape of ferroelectric hysteresis loop has been investigated by TF Analyzer 2000 aixACCT measurement system. It is shown that the remanent polarization and coercive electric field are dependent on the filler volume fraction. Experimental study of ultrasonic wave attenuation, velocity and piezoresponse in these composites has been performed over wide temperature range (100 K – 410 K) using ultrasonic automatic pulseecho technique. The temperature dependences of ultrasonic velocity and attenuation showed anomalies attributed to the glass transition and paraelectric-ferroelectric phase transition.

Saturday, 2015-09-12	09.20	Talk	Ferroic materials and structure	Lecture hall 2

Structural and Magnetic Properties of Mixed Mn–Zn Ferrites Nanoparticles Synthesized by Sol-Gel Method

M. Ben Ali[1,2], K.El Maalam[1,2], H.El Moussaoui[1], O. Mounkachi[1], M. Hamedoun[1], E.K. Hlil[3] and A. Benyoussef[1,2]

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Synthesis and application of magnetic nanoparticles is a subject of intense research because of their unique properties that make them attractive, both from the scientific value of understanding their properties, and the technological significance of enhancing the performance of the existing materials1. Newly, spinel ferrite nanoparticles are regarded as some of the most important inorganic nanomaterials because of their great potential for applications in magnetic resonance imaging 2, drug delivery 2, hyperthermia 2 and newly 3. In this work $Mn_{1-x}Zn_xFe_2O_4$ (x = 0.0 – 0.5) nanoparticles were synthesized through a sol/gel method. The characterization of the synthesized nanoparticle has been done by X-ray diffraction (XRD). The relation between the composition and magnetic properties has been investigated by Magnetic Properties Measurement System (MPMS). The results revealed that the nanocrystals size is in the range of 8 - 9.5 nm. And it was found that the zinc substitution in manganese ferrite increase saturation magnetization from 20 emu/g (x=0) to 61.5 emu/g. Nevertheless, this one decrease after x=0.4 to reach a magnetization equal to 45.5 for x=0.5.

Composites Perovskites Materials for Magnetic Refrigeration Application

K. El Maalam[1, 2], Y. Moubarik[1, 2], O. Mounkachi[1], S. Habouti[4], M. Es-Souni[4], M. Hamedoun[1] and A. Benyoussef[1, 2, 3]

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In this paper a new class of magnetocaloric materials is reported that is based on the composites perovskites $(RE_{0.7}A_{0.3})MnO_3$:CuO (RE=Nd, La…, A = Sr…). Phase purity, structure, size, and crystallinity were investigated using XRD and SEM. Magnetic and magnetocaloric properties of these composites materials have been investigated using different magnetic measurement system.

The Curie temperature is lowered by the Nd substitution when comparing with the La-doped sample. Under an applied field of 1.5 T the maximum values of isothermal entropy change are found to be 2.34, 1.64 J/kg.K for $Nd_{0.7}Sr_{0.3}MnO_3$:5CuO (TC=170 K) and $(La_{0.45}Nd_{0.25})Sr_{0.3}MnO_3$:5CuO (TC=293 K) composites samples, respectiv ely. The phenomenon of large magnetic entropy change and the convenient adjustment of the Curie temperature make the composite perovskite materials useful for magnetic refrigerants in an extended high temperature range even at room temperature.

Saturday, 2015-09-12	10.00	Talk	Ferroic materials and structure	Lecture hall 2

Crystal Structure and Room and High Temperature Raman Spectroscopy Studies of $M_{3-x}M'_xX_2O_8$ (M=Ba, Sr; M'=Pb, Sr; X=P, As, V; 0≤x≤3) and $A_{1-x}A'_xPb_4(XO_4)_3$ (A=Na,K;A'=Ag,K;X=P,As,V and 0≤ x ≤ 1)

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In this work we report on the crystal structure and Raman spectroscopy studies of two large systems:

1- $M_{3-x}M'_xX_2O_8$ (M = Ba, Sr; M' = Pb, Sr; X = P, As, V and 0≤x≤3). The structure consists of XO_4 tetrahedra together with both Ba/Sr/Pb cations occupying statistically two symmetrically distinct sites (the Ba/Sr cations occupy partially two different sites, having either 10- or 12-fold coordination with the oxygen atoms and the same sites are also occupied partially by Pb cations).

Saturday, 2015-09-12	10.00	Talk	Ferroic materials and structure	Lecture hall 2

2- The solid solutions in the system of lead lacunar anionic apatite, $A_{1-x}A'_xPb_4(XO_4)_3$ (A = Na, K; A' = Ag, K; X = P, As, V and $0 \leq x \leq 1$), were successfully synthesized as single phases by solid state method, the final temperature depends on system studied and varies from 550 to 700°C. The samples were characterized by X-ray diffraction, the site of the metal ions (A^+, A'^+ and Pb^{2+}) in the solid solutions was analyzed with the Rietveld method. A variation of the a and c lattice parameters in the solid solutions was observed, with an increase of a and c parameters, related to the radius of the corresponding substituted ions. It was found that Pb ions in the solid solutions preferentially occupied the M(1) and M(2) sites in the lacunar anionic apatite structure. The structure contains channels running along the c axis and centred at (00z). The channels are most probably occupied by the lone electron pairs of the Pb^{2+} cations.

For both systems, Raman spectra of all the compositions are similar for each series and show some linear shifts in band positions as a function of the composition. Assignments of the X–O vibrational stretching and bending modes, as well as some of the external modes, have been made. The temperature dependence of the Raman modes and the corresponding FWHM are studied to detect the existence or not of any temperature induced phase transition.

Saturday, 2015-09-12	10.20	Talk	Ferroic materials and structure	Lecture hall 2

Impedance Complex, Dielectric Relaxation and Electrical Conductivity Studies of $Ba_{1-x}Sr_xTiO_3$ Ceramics

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In this work, we prepared serie of $Ba_{1-x}Sr_xTiO_3$ (BST) powders, with different Strontium concentrations (x =0, 0.025, 0.75, 0.10, 0.125 and 0.15), by sol-gel method. The variation of structure in the system $Ba_{1-x}Sr_xTiO_3$ was analyzed using a combination of XRD and Raman spectroscopy. The field dependence of dielectric relaxation and conductivity was measured over a wide frequency range from room temperature to 400°C. The activation energy, calculated from the temperature dependent to conductivity for different frequency pattern, shows that the Sr has significant effects on the properties of $BaTiO_3$ (The frequency dependence of conductivity was interpreted in terms of the jump of the relaxation model and was fitted by the double power law). Relaxation times extracted using the imaginary part of the impedance complex (Z"(ω)) and the modulus (M"(ω)) were also found following to the Arrhenius law and showed an anomaly around the phase transition temperature.

Saturday, 2015-09-12	11.00	Talk	Ferroic materials and structure	Lecture hall 2

Structural and Electoral Properties of Sol-Gel Processed Strontium–doped Barium Titanate Ceramics

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Sol gel processed Sr-doped barium titanium ceramics, $Ba_{1-x}Sr_xTiO_3$ ($B_{1-x}S_xT$, x=0, 0.1, 0.2, 0.3 and 0.4) were synthesized and characterized using X-ray diffraction (XRD), infrared (FTIR) and Raman techniques. The results show that the samples, for all x, chrystallize in the pseudo-cubic structure. The average crystallite size and other structural parameters were estimated from the XRD patterns. Thermal dielectric (Ɛ') variations indicate a typical phase transition with relatively high values at the temperature of the maximum of Ɛ'. The effect of the Sr concentration on the electrical properties of the BT matrix was examined using the Curie-Weiss law, the power law and the Arrhenius law.

[1] Wei Li, Zhijun Xu, Ruiqing Chu, Peng Fu, Jigong Hao. Structure and electrical properties of $BaTiO_3$ prepared by sol–gel process. Journal of Alloys and Compounds 482 (2009) 137–140
[2] Fengtao Du, Bin Cui, Hualei Cheng, Ruiyuan Niu, Zhuguo Chang. Synthesis, characterization, and dielectric properties of $Ba(Ti_{1\_x}Sn_x)O_3$. Materials Research Bulletin 44 (2009) 1930–1934

Saturday, 2015-09-12	11.20	Talk	Ferroic materials and structure	Lecture hall 2

High Seebeck Coefficients in $ZnO-P_2O_5$/ (Ni & Co) Composites

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The overall purpose of the present study is basically to understand the manifestation of the thermo-electrical properties of the composites $ZnO-P_2O_5$ loaded with different volume fractions of nickel (Ni) and (Co) as conductive fillers. It was shown that the Seebeck coefficient changes from high positive to negative values when the filler amount is increased, indicating a non-conducting to conducting phase transition. Such behavior exhibits that this transition is accompanied by the passing of carrier charge from p to n type. The study of thermoelectrically transport for high volume fraction of filler enabled the achievement, for the first time on this kind of composites, of an original transition called PTC transition. Thus, highest values of power factor ($PF=\sigma S^2 \approx 8x10^{-3} W.m^{-1}.K^{-2}$) were obtained, giving a possibility of industrial applications.

Plenary session

Time: 11.50 – 12.35

Room: Lecture hall 1

Chair: Mohammed Es-Souni

High Performance Hybrid Pseudocapacitive Materials for Energy Storage

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Functional hybrid nanomaterials are of great interest for the fabrication of complex nanoelectronics, optoelectronics and electrochemical devices. In particular, electroactive hybrid nanocomposites are very useful for energy storage based on electrochemical principles, such as supercapacitors or pseudocapacitors. In this talk, we elaborate our efforts on the synthesis of unique hybrid nanocomposites, for example, MnO_2/polyaniline (PANI) and $NiCo_2O_4$/Reduced Graphene Oxide (RGO) suited for high performance supercapacitors. Heterostructures encompassing integrated current collectors such as MnO_2/SnO_2, PANI/ITO and $NiCo(OH)_2$/ZGO will also be discussed from the perspective of reduced contact resistance. In addition, free standing electrodes based on MnO_2/RGO or V_2O_5/RGO have been demonstrated to deliver large areal mass flexible asymmetric supercapacitor with superior performance even under bent condition. The specific capacitance can be enhanced with the shorten ion diffusion length and improved electrochemical active surface of the hybrid paper electrodes. Localized kinetics property at electrolyte/electrode interface was investigated using ultramicroelectrode in the scanning electrochemical microscopy on selected electrode material.

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